

Connecting via Winsock to STN

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LOGINID:ssspat1202txn

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

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NEWS 1      Web Page for STN Seminar Schedule - N. America
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              substances identified in English-, French-, German-,
              and Japanese-language basic patents from 2004-present
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              searching
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NEWS 7 DEC 12 GBFULL now offers single source for full-text
              coverage of complete UK patent families
NEWS 8 DEC 17 Fifty-one pharmaceutical ingredients added to PS
NEWS 9 JAN 06 The retention policy for unread STNmail messages
              will change in 2009 for STN-Columbus and STN-Tokyo
NEWS 10 JAN 07 WPIDS, WPINDEX, and WPIX enhanced Japanese Patent
              Classification Data
NEWS 11 FEB 02 Simultaneous left and right truncation (SLART) added
              for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS 12 FEB 02 GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS 13 FEB 06 Patent sequence location (PSL) data added to USGENE
NEWS 14 FEB 10 COMPENDEX reloaded and enhanced
NEWS 15 FEB 11 WTEXTILES reloaded and enhanced
NEWS 16 FEB 19 New patent-examiner citations in 300,000 CA/CAPLUS
              patent records provide insights into related prior
              art
NEWS 17 FEB 19 Increase the precision of your patent queries -- use
              terms from the IPC Thesaurus, Version 2009.01
NEWS 18 FEB 23 Several formats for image display and print options
              discontinued in USPATFULL and USPAT2
NEWS 19 FEB 23 MEDLINE now offers more precise author group fields
              and 2009 MeSH terms
NEWS 20 FEB 23 TOXCENTER updates mirror those of MEDLINE - more
              precise author group fields and 2009 MeSH terms
NEWS 21 FEB 23 Three million new patent records blast AEROSPACE into
              STN patent clusters

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS   STN Operating Hours Plus Help Desk Availability
NEWS LOGIN   Welcome Banner and News Items
NEWS IPC8    For general information regarding STN implementation of IPC 8

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Enter NEWS followed by the item number or name to see news on that

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specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:39:56 ON 23 FEB 2009

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 11:40:15 ON 23 FEB 2009

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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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STRUCTURE FILE UPDATES: 20 FEB 2009 HIGHEST RN 1109311-46-7

DICTIONARY FILE UPDATES: 20 FEB 2009 HIGHEST RN 1109311-46-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdnoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10562112d.str



```

chain nodes :
7 8 9 10 11 14 28 29 30
ring nodes :
1 2 3 4 5 6 16 17 18 19 20 21 22 23 24 25
chain bonds :
2-7 3-14 6-11 7-8 8-9 8-10 17-29 19-28 24-30
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 20-22
21-25 22-23 23-24 24-25
exact/norm bonds :
2-7 3-14 6-11 7-8 8-9 8-10 16-17 16-21 17-18 17-29 18-19 19-20 19-28
24-30
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 20-21 20-22 21-25 22-23 23-24 24-25

```

G1: Ak, H

G2: H, CN, X

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 14:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 25:Atom 28:CLASS 29:CLASS 30:CLASS
fragments assigned product role:
containing 16
fragments assigned reactant/reagent role:
containing 1

```

L1 STRUCTURE UPLOADED

=> d L1

L1 HAS NO ANSWERS

L1 STR



G1 Ak,H

G2 H,CN,X

Structure attributes must be viewed using STN Express query preparation.

=> file casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.96

1.18

FILE 'CASREACT' ENTERED AT 11:41:31 ON 23 FEB 2009

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FILE CONTENT:1840 - 19 Feb 2009 VOL 150 ISS 2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 16.5 million reactions
*
*
*****
```

CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 11:39:56 ON 23 FEB 2009)

FILE 'REGISTRY' ENTERED AT 11:40:15 ON 23 FEB 2009

L1

STRUCTURE UPLOADED

FILE 'CASREACT' ENTERED AT 11:41:31 ON 23 FEB 2009

> s l1

SAMPLE SEARCH INITIATED 11:41:42 FILE 'CASREACT'
 SCREENING COMPLETE - 2101 REACTIONS TO VERIFY FROM 141 DOCUMENTS
 100.0% DONE 2101 VERIFIED 106 HIT RXNS 12 DOCS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED VERIFICATIONS: 39274 TO 44766
 PROJECTED ANSWERS: 33 TO 447

L2 12 SEA SSS SAM L1 (106 REACTIONS)

> s l1 full

FULL SEARCH INITIATED 11:41:51 FILE 'CASREACT'
 SCREENING COMPLETE - 40457 REACTIONS TO VERIFY FROM 2766 DOCUMENTS
 100.0% DONE 40457 VERIFIED 2129 HIT RXNS 258 DOCS
 SEARCH TIME: 00.00.04

L3 258 SEA SSS FUL L1 (2129 REACTIONS)

> d l3 l- ibib abs hitrxn

'HITRXN' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS ----- GI and AB
 ALL ----- BIB, AB, IND, RE, Single-step Reactions
 APPS ----- AI, PRAI
 BIB ----- AN, plus Bibliographic Data
 CAN ----- List of CA abstract numbers without answer numbers
 CBIB ----- AN, plus Compressed Bibliographic Data
 DALL ----- ALL, delimited (end of each field identified)
 IABS ----- ABS, indented with text labels
 IALL ----- ALL, indented with text labels
 IBIB ----- BIB, indented with text labels
 IND ----- Indexing data
 IPC ----- International Patent Classifications
 ISTD ----- STD, indented with text labels
 OBIB ----- AN, plus Bibliographic Data (original)
 OIBIB ----- OBIB, indented with text labels
 SBIB ----- BIB, no citations
 SIBIB ----- IBIB, no citations
 MAX ----- Same as ALL
 PATS ----- PI, SO
 SCAN ----- TI and FCRD (random display, no answer number. SCAN
 must be entered on the same line as DISPLAY, e.g.,
 D SCAN.)
 SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for
 all single-step reactions)
 STD ----- BIB, IPC, and NCL
 CRD ----- Compact Display of All Hit Reactions
 CRDREF ----- Compact Reaction Display and SO, PY for Reference

FHIT ----- Reaction Map, Diagram, and Summary for first
 hit reaction
 FHITCBIB --- FHIT, AN plus CBIB
 FCRD ----- First hit in Compact Reaction Display (CRD) format
 FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
 CA reference information (SO, PY). (Default)
 FPATH ----- PATH, plus Reaction Summary for the "long path"
 FSPATH ----- SPATH, plus Reaction Summary for the "short path"
 HIT ----- Reaction Map, Reaction Diagram, and Reaction
 Summary for all hit reactions and fields containing
 hit terms
 OCC ----- All hit fields and the number of occurrences of the
 hit terms in each field. Includes total number of
 HIT, PATH, SPATH reactions. Labels reactions that have
 incomplete verifications.
 PATH ----- Reaction Map and Reaction Diagram for the "long
 path". Displays all hit reactions, except those
 whose steps are totally included within another hit
 reaction which is displayed
 RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)
 RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)
 RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
 RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)
 SPATH ----- Reaction Map and Reaction Diagram for the "short
 path". Displays all single step reactions which
 contain a hit substance. Also displays those
 multistep reactions that have a hit substance in both
 the first and last steps of the reaction, except for
 those hit reactions whose steps are totally included
 within another hit reaction which is displayed

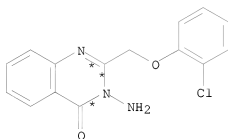
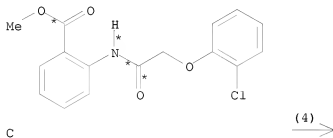
To display a particular field or fields, enter the display field
 codes. For a list of the display field codes, enter HELP DFIELDS
 at an arrow prompt (=>). Examples of combinations include: D TI;
 D BIB RX; D TI, AU, FCRD. The information is displayed in the same order
 as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,
 FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may
 be used with the DISPLAY command to display the record for a specified
 Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):ibib abs rx
 YOU HAVE REQUESTED DATA FROM 258 ANSWERS - CONTINUE? Y/(N):y

L3 ANSWER 1 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 149:402296 CASREACT
 TITLE: Synthesis and antimicrobial activity of some novel
 2,3-disubstituted quinazolin-4(3H)ones
 AUTHOR(S): Abbas, Safinaz E. S.; Saafan, Amal E. M.
 CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of
 Pharmacy, Cairo University, Egypt
 SOURCE: Bulletin of Pharmaceutical Sciences, Assiut University
 (2007), 30(1), 51-62
 CODEN: BPAUEC; ISSN: 1110-0052
 PUBLISHER: Assiut University Press
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 3-Amino-2-(substituted phenoxyethyl/propyl)quinazolin-4(3H)ones (I) have
 been prepared Refluxing I with 5-nitro-2-furaldehyde or 4-nitrobenzaldehyde
 afforded the corresponding methylenediamines. Reaction of I with isatin

yielded the indolyldeneamino derivs. Refluxing I with ofloxacin acid chloride furnished the corresponding carboxamides. Reaction of chloroacetyl chloride with I produced the 3-chloroacetyl amino derivative 9 which upon further reaction with the potassium salts of some antibacterial acids gave the corresponding carboxylate derivs. Sixteen compds. were screened for their antibacterial and antifungal activities. Thirteen compds. were found to possess high to moderate activity against *Pseudomonas aeruginosa* and some of them were also active against *Escherichia coli*. Only one compound was found to exhibit moderate antifungal activity against *Candida albicans*.

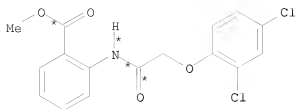
RX(4) OF 60 ...C ==> I...



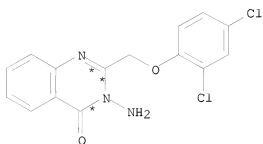
I
YIELD 85%

RX(4) RCT C 301678-87-5
 RGT J 302-01-2 N2H4
 PRO I 1063716-09-5
 SOL 71-36-3 BuOH
 CON 8 - 10 hours, reflux

RX(5) OF 60 ...F ==> L...



F

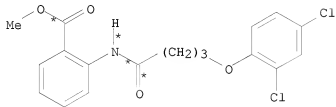
(5) \Rightarrow 

L

YIELD 88%

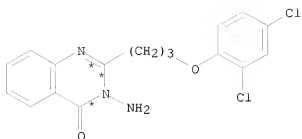
RX(5) RCT F 303794-61-8
 RGT J 302-01-2 N2H4
 PRO L 648859-11-4
 SOL 71-36-3 BuOH
 CON 8 - 10 hours, reflux

RX(6) OF 60 ...H ==> M...



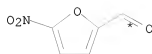
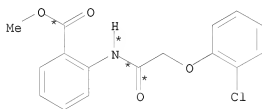
H

(6) \Rightarrow

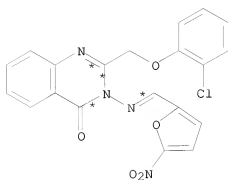


RX(6) RCT H 346724-11-6
RGT J 302-01-2 N2H4
PRO M 1063716-16-4
SOL 71-36-3 BuOH
CON 8 - 10 hours, reflux

RX(26) OF 60 COMPOSED OF RX(4), RX(7)
RX(26) C + N ==> O



2
STEPS
→

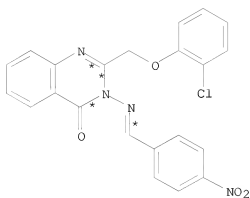
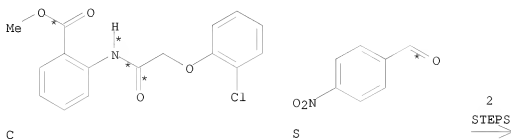


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RX(4) RCT C 301678-87-5
RGT J 302-01-2 N2H4
PRO I 1063716-09-5
SOL 71-36-3 BuOH
CON 8 - 10 hours, reflux

RX(7) RCT I 1063716-09-5, N 698-63-5
PRO O 1063716-20-0
SOL 64-19-7 AcOH
CON 4 hours, reflux
NTE CHEMOSELECTIVE

RX(27) OF 60 COMPOSED OF RX(4), RX(10)
RX(27) C + S ==> T



T
YIELD 72%

RX(4) RCT C 301678-87-5
RGT J 302-01-2 N2H4
PRO I 1063716-09-5
SOL 71-36-3 BuOH
CON 8 - 10 hours, reflux

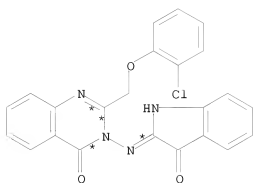
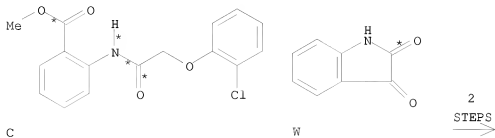
RX(10) RCT I 1063716-09-5, S 555-16-8
PRO T 1063716-34-6
SOL 64-19-7 AcOH
CON 4 hours, reflux

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NTE CHEMOSELECTIVE

RX(28) OF 60 COMPOSED OF RX(4), RX(13)

RX(28) C + W ==> X



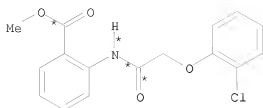
X
YIELD 75%

RX(4) RCT C 301678-87-5
RGT J 302-01-2 N2H4
PRO I 1063716-09-5
SOL 71-36-3 BuOH
CON 8 - 10 hours, reflux

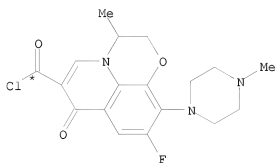
RX(13) RCT I 1063716-09-5, W 91-56-5
PRO X 1063716-48-2
SOL 64-19-7 AcOH
CON 4 - 6 hours, reflux

RX(29) OF 60 COMPOSED OF RX(4), RX(16)

RX(29) C + AA ==> AB



C



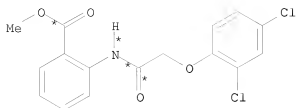
AA

2
STEPS
→

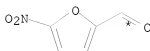
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(4)	RCT	C 301678-87-5
	RGT	J 302-01-2 N2H4
	PRO	I 1063716-09-5
	SOL	71-36-3 BuOH
	CON	8 - 10 hours, reflux
 RX(16)	RCT	I 1063716-09-5, AA 784160-13-0
	RGT	AC 584-08-7 K2CO3
	PRO	AB 1063716-61-9
	SOL	71-43-2 Benzene
	CON	6 hours, reflux

RX(30) OF 60 COMPOSED OF RX(5), RX(8)
RX(30) F + N ==> Q

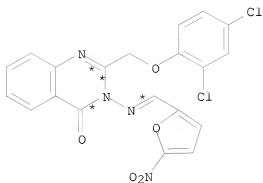


F



N

2
STEPS
→



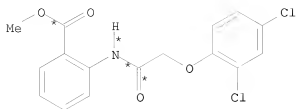
Q
YIELD 73%

RX(5) RCT F 303794-61-8
 RGT J 302-01-2 N2H4
 PRO L 648859-11-4
 SOL 71-36-3 BuOH
 CON 8 - 10 hours, reflux

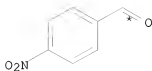
RX(8) RCT L 648859-11-4, N 698-63-5
 PRO Q 1063716-24-4
 SOL 64-19-7 AcOH
 CON 4 hours, reflux
 NTE CHEMOSELECTIVE

RX(31) OF 60 COMPOSED OF RX(5), RX(11)
RX(31) F + S ==> U

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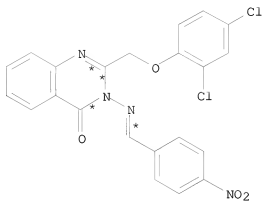


F



S

2
STEPS
→



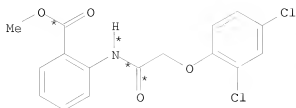
U

YIELD 72%

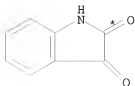
RX(5) RCT F 303794-61-8
 RGT J 302-01-2 N2H4
 PRO L 648859-11-4
 SOL 71-36-3 BuOH
 CON 8 - 10 hours, reflux

RX(11) RCT L 648859-11-4, S 555-16-8
 PRO U 1063716-40-4
 SOL 64-19-7 AcOH
 CON 4 hours, reflux
 NTE CHEMOSELECTIVE

RX(32) OF 60 COMPOSED OF RX(5), RX(14)
 RX(32) F + W ==> Y

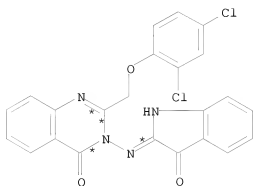


F



W

2
STEPS
→



Y

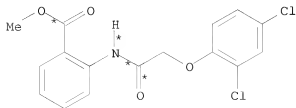
YIELD 72%

RX(5) RCT F 303794-61-8
RGT J 302-01-2 N₂H₄
PRO L 648859-11-4
SOL 71-36-3 BuOH
CON 8 - 10 hours, reflux

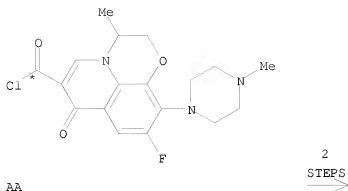
RX(14) RCT L 648859-11-4, W 91-56-5
PRO Y 1063716-53-9
SOL 64-19-7 AcOH
CON 4 - 6 hours, reflux

RX(33) OF 60 COMPOSED OF RX(5), RX(17)

RX(33) F + AA ==> AE



F

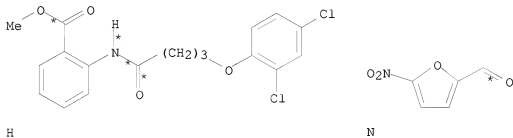


* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(5) RCT F 303794-61-8
 RGT J 302-01-2 N2H4
 PRO L 648859-11-4
 SOL 71-36-3 BuOH
 CON 8 - 10 hours, reflux

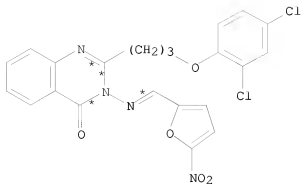
RX(17) RCT L 648859-11-4, AA 784160-13-0
 RGT AC 584-08-7 K2CO3
 PRO AE 1063716-64-2
 SOL 71-43-2 Benzene
 CON 6 hours, reflux

RX(34) OF 60 COMPOSED OF RX(6), RX(9)
 RX(34) H + N ==> R



2
STEPS

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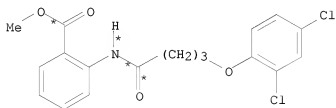
R

YIELD 70%

RX(6) RCT H 346724-11-6
RGT J 302-01-2 N2H4
PRO M 1063716-16-4
SOL 71-36-3 BuOH
CON 8 - 10 hours, reflux

RX(9) RCT M 1063716-16-4, N 698-63-5
PRO R 1063716-29-9
SOL 64-19-7 AcOH
CON 4 hours, reflux
NTE CHEMOSELECTIVE

RX(35) OF 60 COMPOSED OF RX(6), RX(12)
RX(35) H + S ==> V

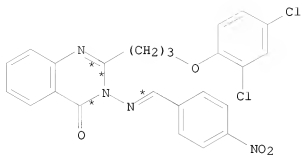


H



S

2
STEPS
=>



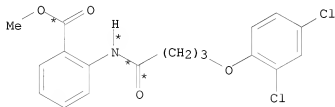
V

YIELD 75%

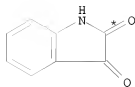
RX(6) RCT H 346724-11-6
 RGT J 302-01-2 N2H4
 PRO M 1063716-16-4
 SOL 71-36-3 BuOH
 CON 8 - 10 hours, reflux

RX(12) RCT M 1063716-16-4, S 555-16-8
 PRO V 1063716-43-7
 SOL 64-19-7 AcOH
 CON 4 hours, reflux
 NTE CHEMOSELECTIVE

RX(36) OF 60 COMPOSED OF RX(6), RX(15)
 RX(36) H + W ==> Z

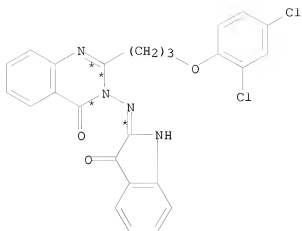


H



W

2
 STEPS
 →

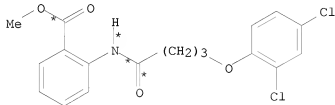


Z
YIELD 70%

RX(6) RCT H 346724-11-6
RGT J 302-01-2 N2H4
PRO M 1063716-16-4
SOL 71-36-3 BuOH
CON 8 - 10 hours, reflux

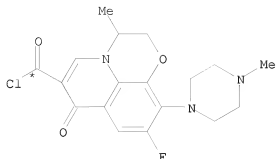
RX(15) RCT M 1063716-16-4, W 91-56-5
PRO Z 1063716-57-3
SOL 64-19-7 AcOH
CON 4 - 6 hours, reflux

RX(37) OF 60 COMPOSED OF RX(6), RX(18)
RX(37) H + AA ==> AF



H

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AA

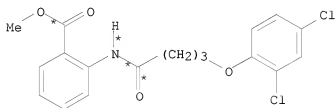
2
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(6) RCT H 346724-11-6
RGT J 302-01-2 N2H4
PRO M 1063716-16-4
SOL 71-36-3 BuOH
CON 8 - 10 hours, reflux

RX(18) RCT M 1063716-16-4, AA 784160-13-0
RGT AC 584-08-7 K2CO3
PRO AF 1063716-67-5
SOL 71-43-2 Benzene
CON 6 hours, reflux

RX(38) OF 60 COMPOSED OF RX(6), RX(19)
RX(38) H + AG ==> AH

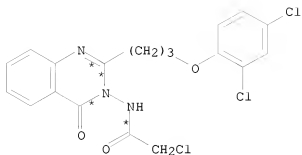


H



AG

2
STEPS
→



AH

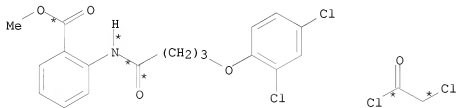
YIELD 80%

RX(6) RCT H 346724-11-6
 RGT J 302-01-2 N2H4
 PRO M 1063716-16-4
 SOL 71-36-3 BuOH
 CON 8 - 10 hours, reflux

 RX(19) RCT M 1063716-16-4, AG 79-04-9
 PRO AH 1063716-70-0
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 2 - 3 hours, room temperature

RX(55) OF 60 COMPOSED OF RX(6), RX(19), RX(20)

RX(55) H + AG + AJ ==> AK



H

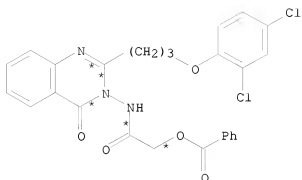
AG



● K

3
STEPS
→

AJ



AK

YIELD 75%

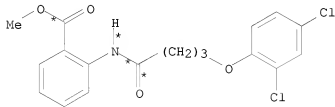
RX(6) RCT H 346724-11-6
 RGT J 302-01-2 N2H4
 PRO M 1063716-16-4
 SOL 71-36-3 BuOH
 CON 8 - 10 hours, reflux

RX(19) RCT M 1063716-16-4, AG 79-04-9
 PRO AH 1063716-70-0
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 2 - 3 hours, room temperature

RX(20) RCT AH 1063716-70-0, AJ 582-25-2
 PRO AK 1063716-72-2
 SOL 68-12-2 DMF
 CON 4 - 6 hours, heated

RX(56) OF 60 COMPOSED OF RX(6), RX(19), RX(21)

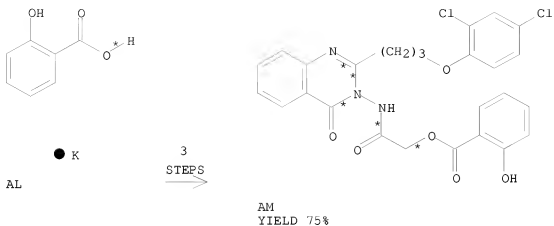
RX(56) H + AG + AL ==> AM



H



AG

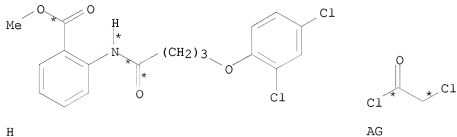


RX(6) RCT H 346724-11-6
 RGT J 302-01-2 N2H4
 PRO M 1063716-16-4
 SOL 71-36-3 BuOH
 CON 8 - 10 hours, reflux

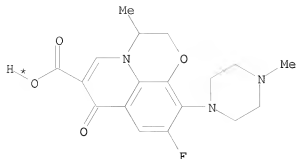
RX(19) RCT M 1063716-16-4, AG 79-04-9
 PRO AH 1063716-70-0
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 2 - 3 hours, room temperature

RX(21) RCT AH 1063716-70-0, AL 578-36-9
 PRO AM 1063716-76-6
 SOL 68-12-2 DMF
 CON 4 - 6 hours, heated

RX(57) OF 60 COMPOSED OF RX(6), RX(19), RX(22)
 RX(57) H + AG + AN ==> AO



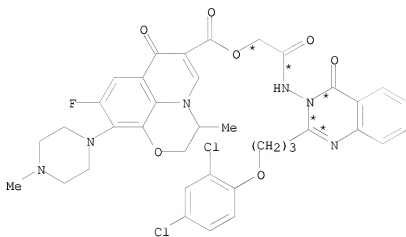
10/ 562,112



● K

3
STEPS
→

AN



AO

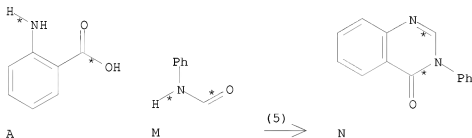
YIELD 70%

RX(6)	RCT	H 346724-11-6
	RGT	J 302-01-2 N2H4
	PRO	M 1063716-16-4
	SOL	71-36-3 BuOH
	CON	8 - 10 hours, reflux
RX(19)	RCT	M 1063716-16-4, AG 79-04-9
	PRO	AH 1063716-70-0
	SOL	68-12-2 DMF
	CON	SUBSTAGE(1) room temperature
		SUBSTAGE(2) 2 - 3 hours, room temperature
RX(22)	RCT	AH 1063716-70-0, AN 1063716-84-6
	PRO	AO 1063716-79-9
	SOL	68-12-2 DMF
	CON	4 - 6 hours, heated

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 149:245729 CASREACT
 TITLE: Anthranilic Acid
 AUTHOR(S): Castedo, Luis; Guitian, Enrique
 CORPORATE SOURCE: Spain
 SOURCE: e-EROS Encyclopedia of Reagents for Organic Synthesis
 (2001), No pp. given. John Wiley & Sons, Ltd.:
 Chichester, UK.
 CODEN: 69KUHI
 URL: <http://www3.interscience.wiley.com/cgi-bin/mrwhome/104554785/HOME>
 DOCUMENT TYPE: Conference; General Review; (online computer file)
 LANGUAGE: English
 AB A review of the article Anthranilic Acid.

RX(5) OF 5 A + M ==> N



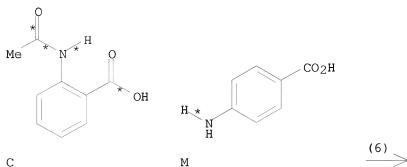
RX(5) RCT A 118-92-3, M 103-70-8
 PRO N 16347-60-7
 CON 130 deg C
 NTE Synthesis of Heterocycles

L3 ANSWER 3 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 148:538299 CASREACT
 TITLE: Process for synthesis of quinazolinones as
 antimycobacterial agents
 INVENTOR(S): Meyyanathan, S. N.; Suresh, Bhojraj; Anbunathan,
 Perumal Nirmala
 PATENT ASSIGNEE(S): India
 SOURCE: Indian Pat. Appl., 14pp.
 CODEN: INXXBQ
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 2004CH01048	A	20070309	IN 2004-CH1048	20041011

PRIORITY APPLN. INFO.:
 OTHER SOURCE(S): MARPAT 148:538299
 AB A process for the synthesis of 4-(2-methyl-4-oxo-4h-quinazolin-3-yl)-benzoyl pyrrolidine-2-carboxylic acid starting from anthranilic acids and acetic anhydride. The claimed compds. are active against Mycobacterium tuberculosis.

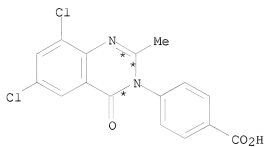
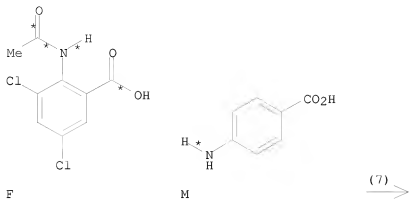
RX(6) OF 44 ...C + M ==> N...



N
 YIELD 93%

RX(6) RCT C 89-52-1, M 150-13-0
 RGT O 64-19-7 AcOH, P 1314-56-3 P205
 PRO N 4005-05-4
 SOL 7732-18-5 Water
 CON 6 hours, reflux

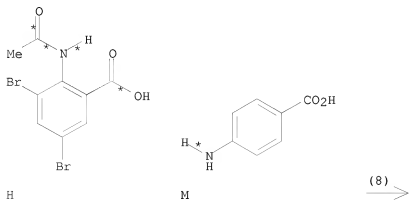
RX(7) OF 44 ...F + M ==> R...

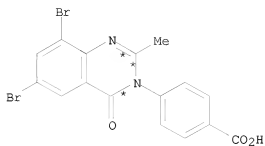


R
YIELD 89%

RX(7) RCT F 19094-64-5, M 150-13-0
RGT O 64-19-7 AcOH, P 1314-56-3 P2O5
PRO R 1023888-34-7
SOL 7732-18-5 Water
CON 8.5 hours, reflux

RX(8) OF 44 ...H + M ==> S...

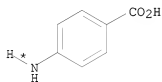




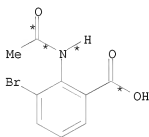
S
YIELD 100%

RX(8) RCT H 16610-45-0, M 150-13-0
 RGT O 64-19-7 AcOH, P 1314-56-3 P205
 PRO S 24295-52-1
 SOL 7732-18-5 Water
 CON 5.5 hours, reflux

RX(9) OF 44 M + T ==> U...

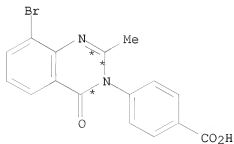


M



T

(9) →

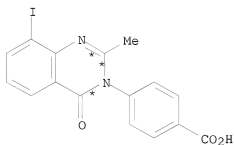
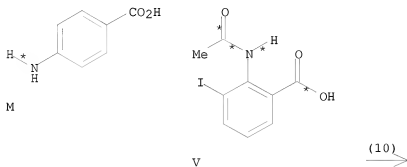


U
YIELD 93%

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RX(9) RCT M 150-13-0, T 861791-77-7
 RGT O 64-19-7 AcOH, P 1314-56-3 P205
 PRO U 1023888-35-8
 SOL 7732-18-5 Water
 CON 5.5 hours, reflux

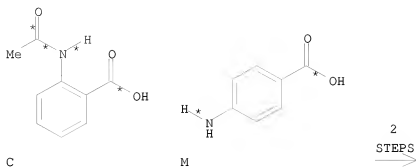
RX(10) OF 44 M + V ==> W...



YIELD 100%

RX(10) RCT M 150-13-0, V 1027340-18-6
 RGT O 64-19-7 AcOH, P 1314-56-3 P205
 PRO W 1023888-36-9
 SOL 7732-18-5 Water
 CON 3 hours, reflux

RX(24) OF 44 COMPOSED OF RX(6), RX(11)
 RX(24) C + M ==> X



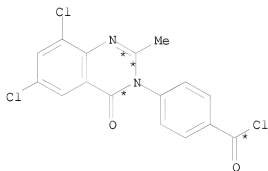
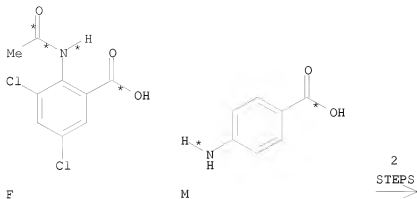
X
YIELD 85%

RX(6) RCT C 89-52-1, M 150-13-0
RGT O 64-19-7 AcOH, P 1314-56-3 P205
PRO N 4005-05-4
SOL 7732-18-5 Water
CON 6 hours, reflux

RX(11) RCT N 4005-05-4
RGT Y 7719-09-7 SOCl2
PRO X 863988-62-9
SOL 123-91-1 Dioxane
CON 4 hours, reflux

RX(25) OF 44 COMPOSED OF RX(7), RX(12)
RX(25) F + M ==> AA

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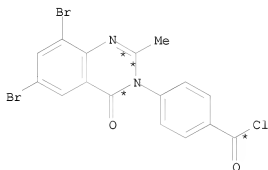
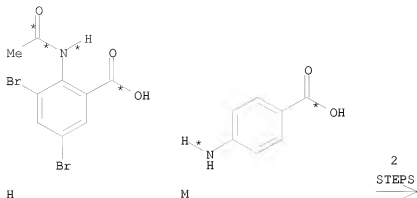
AA
YIELD 82%

RX(7) RCT F 19094-64-5, M 150-13-0
 RGT O 64-19-7 AcOH, P 1314-56-3 P205
 PRO R 1023888-34-7
 SOL 7732-18-5 Water
 CON 8.5 hours, reflux

RX(12) RCT R 1023888-34-7
 RGT Y 7719-09-7 SOCl2
 PRO AA 1023888-37-0
 SOL 123-91-1 Dioxane
 CON 6 hours, reflux

RX(26) OF 44 COMPOSED OF RX(8), RX(13)
 RX(26) H + M ==> AB

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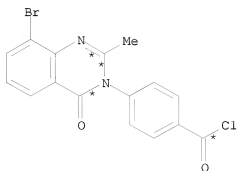
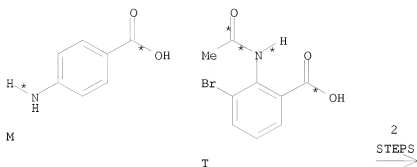


AB
YIELD 77%

RX(8) RCT H 16610-45-0, M 150-13-0
RGT O 64-19-7 AcOH, P 1314-56-3 P205
PRO S 24295-52-1
SOL 7732-18-5 Water
CON 5.5 hours, reflux

RX(13) RCT S 24295-52-1
RGT Y 7719-09-7 SOCl2
PRO AB 1023888-38-1
SOL 123-91-1 Dioxane
CON 6.25 hours, reflux

RX(27) OF 44 COMPOSED OF RX(9), RX(14)
RX(27) M + T ==> AC

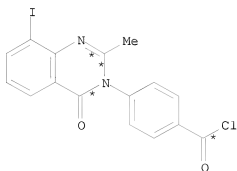
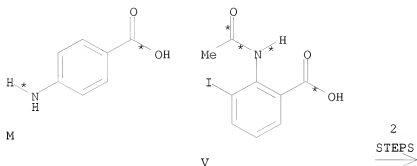


AC
YIELD 97%

RX(9) RCT M 150-13-0, T 861791-77-7
 RGT O 64-19-7 AcOH, P 1314-56-3 P2O5
 PRO U 1023888-35-8
 SOL 7732-18-5 Water
 CON 5.5 hours, reflux

RX(14) RCT U 1023888-35-8
 RGT Y 7719-09-7 SOCl2
 PRO AC 1023888-39-2
 SOL 123-91-1 Dioxane
 CON 10 hours, reflux

RX(28) OF 44 COMPOSED OF RX(10), RX(15)
 RX(28) M + V ==> AD

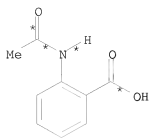


AD
YIELD 60%

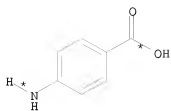
RX(10) RCT M 150-13-0, V 1027340-18-6
 RGT O 64-19-7 AcOH, P 1314-56-3 P2O5
 PRO W 1023888-36-9
 SOL 7732-18-5 Water
 CON 3 hours, reflux

RX(15) RCT W 1023888-36-9
 RGT Y 7719-09-7 SOCl2
 PRO AD 1023888-40-5
 SOL 123-91-1 Dioxane
 CON 7.5 hours, reflux

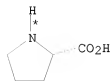
RX(37) OF 44 COMPOSED OF RX(6), RX(11), RX(16)
 RX(37) C + M + AE ==> AF



C

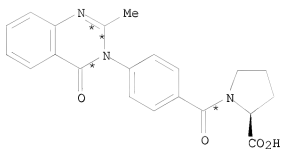


M



AE

3
STEPS
→



AF
YIELD 66%

```

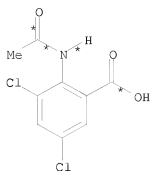
RX(6)      RCT  C 89-52-1, M 150-13-0
           RGT  O 64-19-7 AcOH, P 1314-56-3 P205
           PRO  N 4005-05-4
           SOL  7732-18-5 Water
           CON  6 hours, reflux

RX(11)     RCT  N 4005-05-4
           RGT  Y 7719-09-7 SOCl2
           PRO  X 863988-62-9
           SOL  123-91-1 Dioxane
           CON  4 hours, reflux

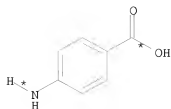
RX(16)     RCT  X 863988-62-9, AE 147-85-3
           RGT  AG 1310-73-2 NaOH
           PRO  AF 1023888-41-6
           SOL  7732-18-5 Water, 123-91-1 Dioxane
           CON  6 hours, reflux

RX(39) OF  44 COMPOSED OF RX(7), RX(12), RX(17)
RX(39)     F  +  M  +  AE  ==>  AH
  
```

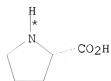
10/ 562,112



F

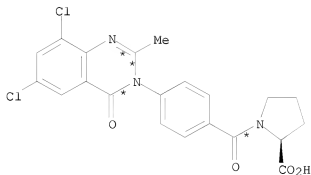


M



AE

3
STEPS
→



AH
YIELD 63%

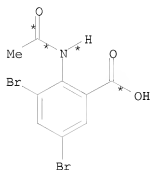
RX(7) RCT F 19094-64-5, M 150-13-0
RGT O 64-19-7 AcOH, P 1314-56-3 P205
PRO R 1023888-34-7
SOL 7732-18-5 Water
CON 8.5 hours, reflux

RX(12) RCT R 1023888-34-7
RGT Y 7719-09-7 SOC12
PRO AA 1023888-37-0
SOL 123-91-1 Dioxane
CON 6 hours, reflux

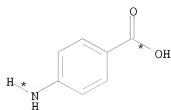
RX(17) RCT AA 1023888-37-0, AE 147-85-3
RGT AG 1310-73-2 NaOH
PRO AH 1023888-42-7
SOL 7732-18-5 Water, 123-91-1 Dioxane
CON 10.25 hours, reflux

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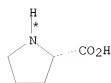
RX(41) OF 44 COMPOSED OF RX(8), RX(13), RX(18)
 RX(41) H + M + AE ==> AI



H

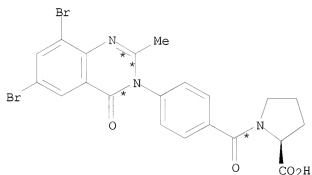


M



AE

3
 STEPS
 →



AI
 YIELD 88%

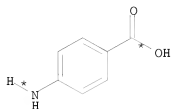
RX(8)	RCT	H 16610-45-0, M 150-13-0
	RGT	O 64-19-7 AcOH, P 1314-56-3 P205
	PRO	S 24295-52-1
	SOL	7732-18-5 Water
	CON	5.5 hours, reflux
RX(13)	RCT	S 24295-52-1
	RGT	Y 7719-09-7 SOCl2
	PRO	AB 1023888-38-1
	SOL	123-91-1 Dioxane
	CON	6.25 hours, reflux
RX(18)	RCT	AB 1023888-38-1, AE 147-85-3
	RGT	AG 1310-73-2 NaOH
	PRO	AI 1023888-43-8
	SOL	7732-18-5 Water, 123-91-1 Dioxane

10/ 562,112

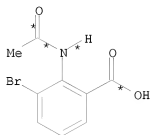
CON 8 hours, reflux

RX(43) OF 44 COMPOSED OF RX(9), RX(14), RX(19)

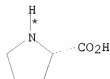
RX(43) M + T + AE ==> AJ



M

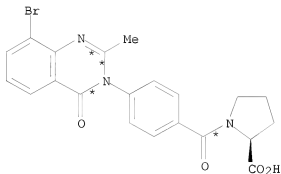


T



AE

3
STEPS
→



AJ

YIELD 86%

RX(9) RCT M 150-13-0, T 861791-77-7
RGT O 64-19-7 AcOH, P 1314-56-3 P205
PRO U 1023888-35-8
SOL 7732-18-5 Water
CON 5.5 hours, reflux

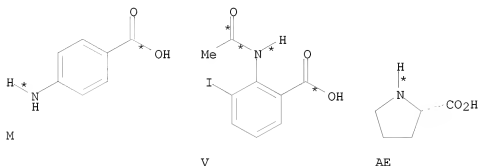
RX(14) RCT U 1023888-35-8
RGT Y 7719-09-7 SOCl2
PRO AC 1023888-39-2
SOL 123-91-1 Dioxane
CON 10 hours, reflux

RX(19) RCT AC 1023888-39-2, AE 147-85-3
RGT AG 1310-73-2 NaOH
PRO AJ 1023888-44-9

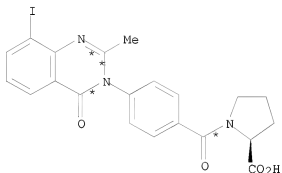
10/ 562,112

SOL 7732-18-5 Water, 123-91-1 Dioxane
CON 8 hours, reflux

RX(44) OF 44 COMPOSED OF RX(10), RX(15), RX(20)
RX(44) M + V + AE ==> AK



3
STEPS
→



AK
YIELD 57%

RX(10) RCT M 150-13-0, V 1027340-18-6
RGT O 64-19-7 AcOH, P 1314-56-3 P205
PRO W 1023888-36-9
SOL 7732-18-5 Water
CON 3 hours, reflux

RX(15) RCT W 1023888-36-9
RGT Y 7719-09-7 SOCl2
PRO AD 1023888-40-5
SOL 123-91-1 Dioxane
CON 7.5 hours, reflux

RX(20) RCT AD 1023888-40-5, AE 147-85-3
RGT AG 1310-73-2 NaOH

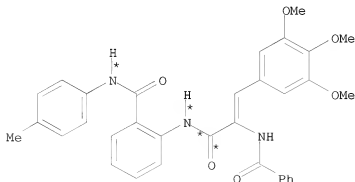
PRO AK 1023888-45-0
 SOL 7732-18-5 Water, 123-91-1 Dioxane
 CON 10.75 hours, reflux

L3 ANSWER 4 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 148:495870 CASREACT
 TITLE: Synthesis of new thiadiazoles,
 1,2,4-triazolo[3,4-b]-1,3,4-thiadiazoles, and
 1,2,4-triazolo[2,3-c]quinazoline derivatives from
 4H-3,1-benzoxazin-4-one derivative
 AUTHOR(S): Mahmoud, M. R.; El-Bordany, E. A.; Azab, M. E.;
 Soliman, E. A.
 CORPORATE SOURCE: Chemistry Department, Ain Shams University, Cairo,
 Egypt
 SOURCE: Phosphorus, Sulfur and Silicon and the Related
 Elements (2007), 182(6), 1275-1289
 CODEN: PSSLEC; ISSN: 1042-6507
 PUBLISHER: Taylor & Francis, Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 4H-3,1-benzoxazin-4-one derivative (I) was reacted with Grignard reagents, primary and secondary amines, glycine, hydrazine hydrate, azines, and a Schiff base. The acid hydrazide derivative (II) was the key starting material for the synthesis of triazole, triazolo[3,4-b]thiadiazole, thiadiazole, and triazolo[2,3-c]quinazoline derivs., e.g., III and IV.

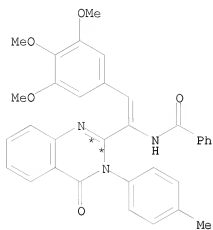
RX(24) OF 69 ...AY ==> BB



AY

(24) →

10/ 562,112

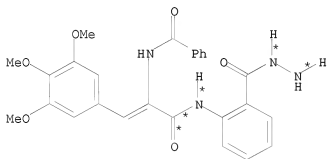


BB

YIELD 70%

RX(24) RCT AY 1020730-48-6
 PRO BB 1020730-49-7
 CON SUBSTAGE(1) 1 hour, 200 deg C
 SUBSTAGE(2) cooled

RX(26) OF 69 ...AE + BD ==> BE

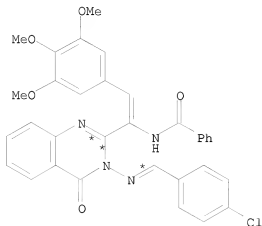


AE



BD

(26)



BE

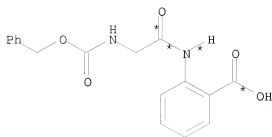
RX(26) RCT AE 1020730-27-1, BD 104-88-1
 RGT BC 127-09-3 AcONa
 PRO BE 1020730-50-0
 SOL 64-19-7 AcOH
 CON 3 hours, reflux

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

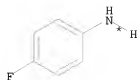
L3 ANSWER 5 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 148:417239 CASREACT
 TITLE: Potent Inhibitors of the Hedgehog Signaling Pathway
 AUTHOR(S): Brunton, Shirley A.; Stibbard, John H. A.; Rubin, Lee L.; Kruse, Lawrence I.; Guicherit, Oivin M.; Boyd, Edward A.; Price, Steven
 CORPORATE SOURCE: Evotec, Abingdon, Oxfordshire, OX14 4RX, UK
 SOURCE: Journal of Medicinal Chemistry (2008), 51(5), 1108-1110
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A small family of Ph quinazolinone ureas is reported as potent modulators of Hedgehog protein function. Preliminary SAR studies of the urea substituent led to a nanomolar Hedgehog antagonist.

RX(12) OF 105 ...AG + AJ ==> AK...

10/ 562,112

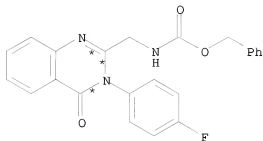


AG



AJ

(12)



AK

YIELD 48%

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone

SOL 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4

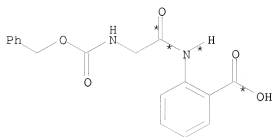
SOL 109-99-9 THF

CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

RX(27) OF 105 ...AG + BQ ==> BP...

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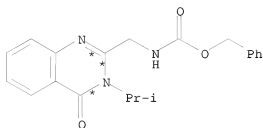


AG



BQ

(27) →



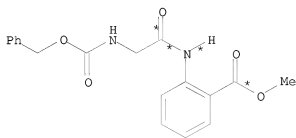
BP

YIELD 48%

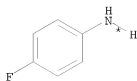
RX(27) RCT AG 55301-19-4, BQ 75-31-0
 RGT AE 530-62-1 Diimidazolyl ketone
 PRO BP 1072784-96-3
 SOL 109-99-9 THF
 CON 20 hours, reflux

RX(35) OF 105 COMPOSED OF RX(11), RX(12)

RX(35) AD + AJ ==> AK



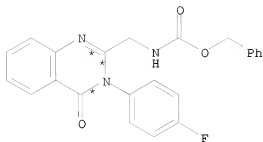
AD



AJ

2
 STEPS
 →

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AK

YIELD 48%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH

SOL 7732-18-5 Water, 123-91-1 Dioxane

CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

CON pH 1

PRO AG 55301-19-4

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone

SOL 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4

SOL 109-99-9 THF

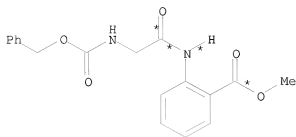
CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

RX(36) OF 105 COMPOSED OF RX(11), RX(27)

RX(36) AD + BQ ==> BP

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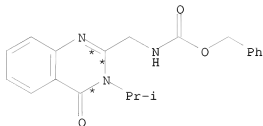


AD



BQ

2
STEPS
➤



BP

YIELD 48%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH

SOL 7732-18-5 Water, 123-91-1 Dioxane

CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

CON pH 1

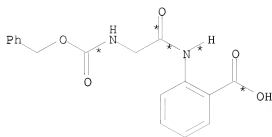
PRO AG 55301-19-4

RX(27) RCT AG 55301-19-4, BQ 75-31-0
RGT AE 530-62-1 Diimidazolyl ketone
PRO BP 1072784-96-3
SOL 109-99-9 THF
CON 20 hours, reflux

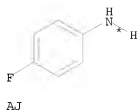
RX(37) OF 105 COMPOSED OF RX(12), RX(13)

RX(37) AG + AJ ==> AL

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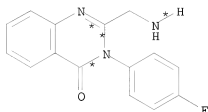


AG



AJ

2
STEPS
→



AL

YIELD 95%

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone

SOL 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4

SOL 109-99-9 THF

CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0

RGT AM 1333-74-0 H2

PRO AL 330796-23-1

CAT 7440-05-3 Pd

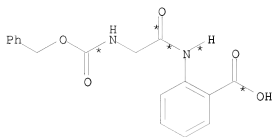
SOL 64-17-5 EtOH

CON 2 hours, room temperature

RX(51) OF 105 COMPOSED OF RX(27), RX(26)

RX(51) AG + BQ ==> R

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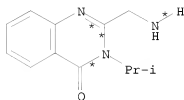


AG



BQ

2
STEPS
→



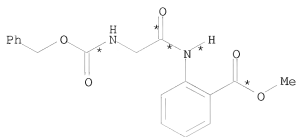
R
YIELD 95%

RX(27) RCT AG 55301-19-4, BQ 75-31-0
RGT AE 530-62-1 Diimidazolyl ketone
PRO BP 1072784-96-3
SOL 109-99-9 THF
CON 20 hours, reflux

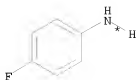
RX(26) RCT BP 1072784-96-3
RGT AM 1333-74-0 H2
PRO R 1072784-05-4
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH
CON 2 hours, room temperature

RX(64) OF 105 COMPOSED OF RX(11), RX(12), RX(13)
RX(64) AD + AJ ==> AL

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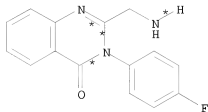


AD



AJ

3
STEPS
➤



AL
YIELD 95%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH
SOL 7732-18-5 Water, 123-91-1 Dioxane
CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
CON pH 1

PRO AG 55301-19-4

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone
SOL 109-99-9 THF
CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4
SOL 109-99-9 THF
CON 20 hours, room temperature -> 70 deg C

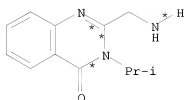
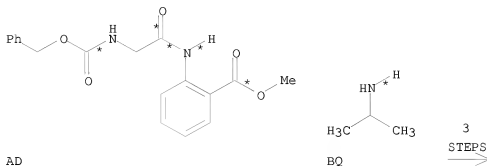
PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0

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RGT AM 1333-74-0 H2
PRO AL 330796-23-1
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH
CON 2 hours, room temperature

RX(65) OF 105 COMPOSED OF RX(11), RX(27), RX(26)
RX(65) AD + BQ ==> R



YIELD 95%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH
SOL 7732-18-5 Water, 123-91-1 Dioxane
CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
CON pH 1

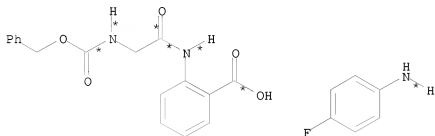
PRO AG 55301-19-4

RX(27) RCT AG 55301-19-4, BQ 75-31-0
RGT AE 530-62-1 Diimidazolyl ketone
PRO BP 1072784-96-3
SOL 109-99-9 THF
CON 20 hours, reflux

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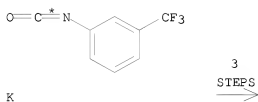
RX(26) RCT BP 1072784-96-3
RGT AM 1333-74-0 H2
PRO R 1072784-05-4
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH
CON 2 hours, room temperature

RX(68) OF 105 COMPOSED OF RX(12), RX(13), RX(14)
RX(68) AG + AJ + K ==> AO



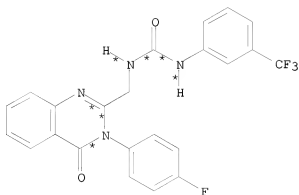
AG

AJ



K

3
STEPS
=>



AO
YIELD 65%

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone
 SOL 109-99-9 THF
 CON 1 hour, room temperature

STAGE(2)

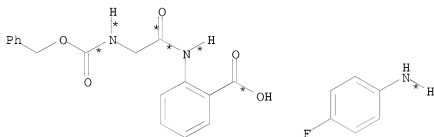
RCT AJ 371-40-4
 SOL 109-99-9 THF
 CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0
 RGT AM 1333-74-0 H2
 PRO AL 330796-23-1
 CAT 7440-05-3 Pd
 SOL 64-17-5 EtOH
 CON 2 hours, room temperature

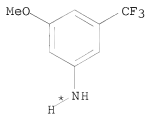
RX(14) RCT K 329-01-1, AL 330796-23-1
 PRO AO 330796-21-9
 SOL 75-09-2 CH2Cl2
 CON 3 hours, room temperature

RX(69) OF 105 COMPOSED OF RX(12), RX(13), RX(15)
 RX(69) AG + AJ + AQ + AR ==> AS

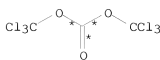


AG

AJ

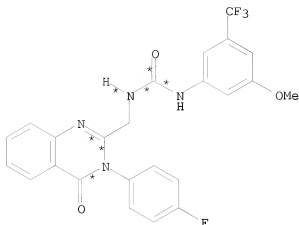


AQ



AR

3
STEPS
→



AS
YIELD 24%

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone
SOL 109-99-9 THF
CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4
SOL 109-99-9 THF
CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0
RGT AM 1333-74-0 H2
PRO AL 330796-23-1
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH
CON 2 hours, room temperature

RX(15) RCT AQ 349-55-3, AR 32315-10-9

STAGE(1)

CAT 7440-44-0 Carbon
SOL 141-78-6 AcOEt
CON 2 hours, room temperature -> 78 deg C

STAGE(2)

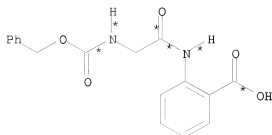
RCT AL 330796-23-1
SOL 67-66-3 CHCl3
CON 18 hours, room temperature

PRO AS 1016901-87-3

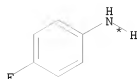
RX(70) OF 105 COMPOSED OF RX(12), RX(13), RX(16)

10/ 562,112

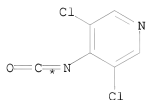
RX(70) AG + AJ + AV ==> AW



AG

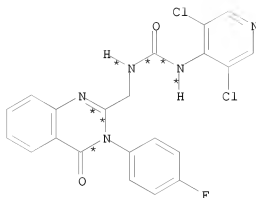


AJ



AV

3
STEPS
→



AW
YIELD 96%

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone

SOL 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4

SOL 109-99-9 THF

CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

RX(13)

RCT AK 330796-22-0

RGT AM 1333-74-0 H2

PRO AL 330796-23-1

CAT 7440-05-3 Pd

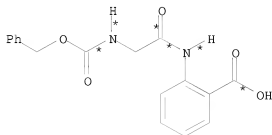
SOL 64-17-5 EtOH

CON 2 hours, room temperature

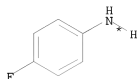
10/ 562,112

RX(16) RCT AL 330796-23-1, AV 481704-32-9
PRO AW 1016901-88-4
SOL 75-09-2 CH2Cl2
CON 3 hours, room temperature

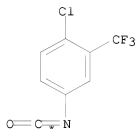
RX(71) OF 105 COMPOSED OF RX(12), RX(13), RX(17)
RX(71) AG + AJ + AX ==> AY



AG

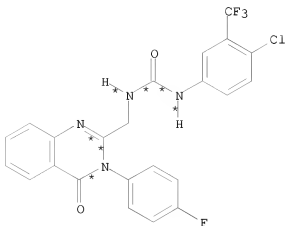


AJ



AX

3
STEPS
→



AY
YIELD 100%

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone
SOL 109-99-9 THF
CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4
SOL 109-99-9 THF
CON 20 hours, room temperature -> 70 deg C

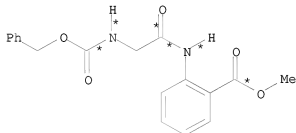
10/ 562,112

PRO AK 330796-22-0

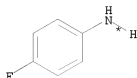
RX(13) RCT AK 330796-22-0
 RGT AM 1333-74-0 H2
 PRO AL 330796-23-1
 CAT 7440-05-3 Pd
 SOL 64-17-5 EtOH
 CON 2 hours, room temperature

RX(17) RCT AL 330796-23-1, AX 327-78-6
 PRO AY 330796-24-2
 SOL 75-09-2 CH2Cl2
 CON 3 hours, room temperature

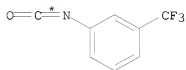
RX(72) OF 105 COMPOSED OF RX(11), RX(12), RX(13), RX(14)
 RX(72) AD + AJ + K ==> AO



AD

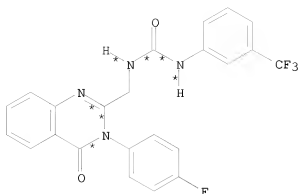


AJ



K

4
 STEPS
 →



AO
YIELD 65%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH
SOL 7732-18-5 Water, 123-91-1 Dioxane
CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
CON pH 1

PRO AG 55301-19-4

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone
SOL 109-99-9 THF
CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4
SOL 109-99-9 THF
CON 20 hours, room temperature -> 70 deg C

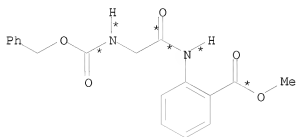
PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0
RGT AM 1333-74-0 H2
PRO AL 330796-23-1
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH
CON 2 hours, room temperature

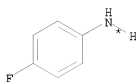
RX(14) RCT K 329-01-1, AL 330796-23-1
PRO AO 330796-21-9
SOL 75-09-2 CH2Cl2
CON 3 hours, room temperature

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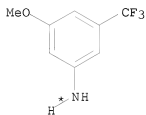
RX(73) OF 105 COMPOSED OF RX(11), RX(12), RX(13), RX(15)
 RX(73) AD + AJ + AQ + AR ==> AS



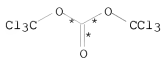
AD



AJ

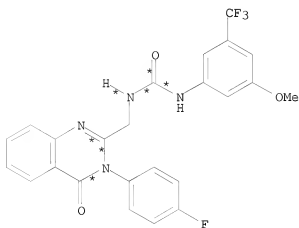


AQ



AR

4
STEPS
→



AS

YIELD 24%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH

10/ 562,112

SOL 7732-18-5 Water, 123-91-1 Dioxane
CON 18 hours, room temperature

STAGE(2)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
CON pH 1

PRO AG 55301-19-4

RX(12) RCT AG 55301-19-4

STAGE(1)
RGT AE 530-62-1 Diimidazolyl ketone
SOL 109-99-9 THF
CON 1 hour, room temperature

STAGE(2)
RCT AJ 371-40-4
SOL 109-99-9 THF
CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0
RGT AM 1333-74-0 H2
PRO AL 330796-23-1
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH
CON 2 hours, room temperature

RX(15) RCT AQ 349-55-3, AR 32315-10-9

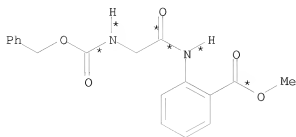
STAGE(1)
CAT 7440-44-0 Carbon
SOL 141-78-6 AcOEt
CON 2 hours, room temperature -> 78 deg C

STAGE(2)
RCT AL 330796-23-1
SOL 67-66-3 CHCl3
CON 18 hours, room temperature

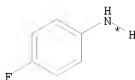
PRO AS 1016901-87-3

RX(74) OF 105 COMPOSED OF RX(11), RX(12), RX(13), RX(16)

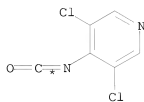
RX(74) AD + AJ + AV ==> AW



AD

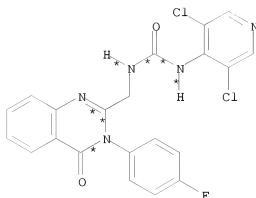


AJ



AV

4
STEPS
→



AW
YIELD 96%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH

SOL 7732-18-5 Water, 123-91-1 Dioxane

CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

CON pH 1

PRO AG 55301-19-4

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone

SOL 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RCT AJ 371-40-4

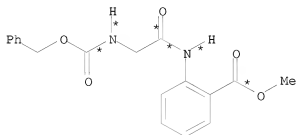
SOL 109-99-9 THF
 CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

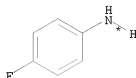
RX(13) RCT AK 330796-22-0
 RGT AM 1333-74-0 H2
 PRO AL 330796-23-1
 CAT 7440-05-3 Pd
 SOL 64-17-5 EtOH
 CON 2 hours, room temperature

RX(16) RCT AL 330796-23-1, AV 481704-32-9
 PRO AW 1016901-88-4
 SOL 75-09-2 CH2Cl2
 CON 3 hours, room temperature

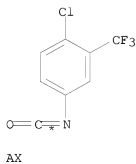
RX(75) OF 105 COMPOSED OF RX(11), RX(12), RX(13), RX(17)
 RX(75) AD + AJ + AX ==> AY



AD

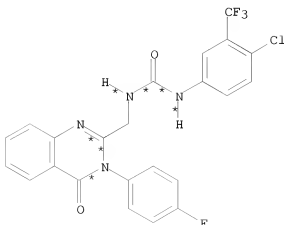


AJ



AX

4
 STEPS
 →



AY
 YIELD 100%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH
 SOL 7732-18-5 Water, 123-91-1 Dioxane
 CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON pH 1

PRO AG 55301-19-4

RX(12) RCT AG 55301-19-4

STAGE(1)

RGT AE 530-62-1 Diimidazolyl ketone
 SOL 109-99-9 THF
 CON 1 hour, room temperature

STAGE(2)

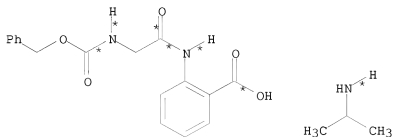
RCT AJ 371-40-4
 SOL 109-99-9 THF
 CON 20 hours, room temperature -> 70 deg C

PRO AK 330796-22-0

RX(13) RCT AK 330796-22-0
 RGT AM 1333-74-0 H2
 PRO AL 330796-23-1
 CAT 7440-05-3 Pd
 SOL 64-17-5 EtOH
 CON 2 hours, room temperature

RX(17) RCT AL 330796-23-1, AX 327-78-6
 PRO AY 330796-24-2
 SOL 75-09-2 CH2Cl2
 CON 3 hours, room temperature

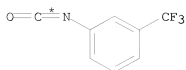
RX(85) OF 105 COMPOSED OF RX(27), RX(26), RX(6)
 RX(85) AG + BQ + K ==> S



AG

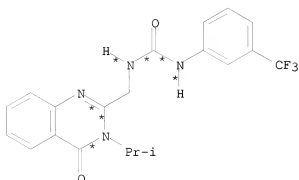
BQ

10/ 562,112



K

3
STEPS
→



S

YIELD 11%

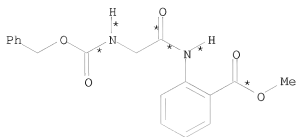
RX(27) RCT AG 55301-19-4, BQ 75-31-0
RGT AE 530-62-1 Diimidazolyl ketone
PRO BP 1072784-96-3
SOL 109-99-9 THF
CON 20 hours, reflux

RX(26) RCT BP 1072784-96-3
RGT AM 1333-74-0 H2
PRO R 1072784-05-4
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH
CON 2 hours, room temperature

RX(6) RCT K 329-01-1, R 1072784-05-4
PRO S 1016901-86-2
SOL 67-66-3 CHCl3
CON SUBSTAGE(1) 10 minutes, 0 deg C
SUBSTAGE(2) 1 hour, 0 deg C

RX(86) OF 105 COMPOSED OF RX(11), RX(27), RX(26), RX(6)
RX(86) AD + BQ + K ==> S

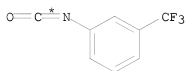
10/ 562,112



AD

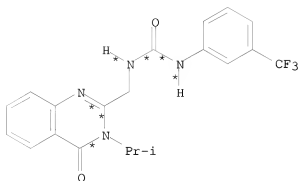


BQ



K

4
STEPS
→



S

YIELD 11%

RX(11) RCT AD 133010-41-0

STAGE(1)

RGT AH 1310-65-2 LiOH
SOL 7732-18-5 Water, 123-91-1 Dioxane
CON 18 hours, room temperature

STAGE(2)

RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
CON pH 1

PRO AG 55301-19-4

RX(27) RCT AG 55301-19-4, BQ 75-31-0
 RGT AE 530-62-1 Diimidazolyl ketone
 PRO BP 1072784-96-3
 SOL 109-99-9 THF
 CON 20 hours, reflux

RX(26) RCT BP 1072784-96-3
 RGT AM 1333-74-0 H2
 PRO R 1072784-05-4
 CAT 7440-05-3 Pd
 SOL 64-17-5 EtOH
 CON 2 hours, room temperature

RX(6) RCT K 329-01-1, R 1072784-05-4
 PRO S 1016901-86-2
 SOL 67-66-3 CHCl3
 CON SUBSTAGE(1) 10 minutes, 0 deg C
 SUBSTAGE(2) 1 hour, 0 deg C

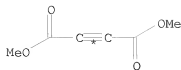
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

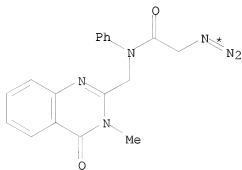
ACCESSION NUMBER: 148:379548 CASREACT
 TITLE: Bisheterocycles: synthesis of some novel
 1,2,3-triazolyloxadiazole and -4(3H)-quinazolinones
 via azide cycloaddition reaction
 AUTHOR(S): Komaraiah, A.; Ramakrishna, K.; Sailu, B.; Reddy, P.
 S. N.
 CORPORATE SOURCE: Department of Chemistry, Osmania University,
 Hyderabad, 500007, India
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2007), (14),
 110-116
 CODEN: AGFUAR
 URL: http://content.arkat-usa.org/ARKIVOC/JOURNAL_CONTENT/manuscripts/2007/07-2388MP%20as%20published%20mainmanuscript.pdf
 PUBLISHER: Arkat USA Inc.
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English
 AB 2,5-Bis[2-(4,5-dimethoxycarbonyl)1,2,3-triazol-1-ylacetylaminophenyl]-
 1,3,4-oxadiazole and di-Me 1-(2-((3-methyl-4-oxo-3,4-dihydro-2-
 quinazolinyl)methyl)anilino)-2-oxoethyl)-1H-1,2,3-triazole-4,5-
 dicarboxylate are prepared by cycloaddn. of di-Me acetylenedicarboxylate to
 2,5-bis(2-azidoacetylaminophenyl)1,3,4-oxadiazole and
 2-(N-aryl-N-azidoacetylaminomethyl)-3-methylquinazolin-4-one, resp.

RX(4) OF 11 H + K ==> L

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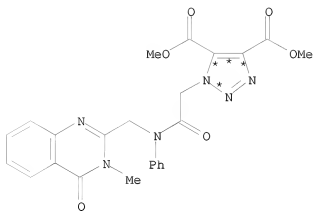


H



K

(4) →



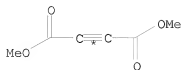
L

YIELD 74%

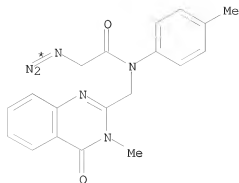
RX(4)	RCT	H 762-42-5, K 536697-61-7
	PRO	L 1014987-15-5
	SOL	67-64-1 Me2CO
	CON	12 - 14 hours, reflux

RX(5) OF 11 H + M ==> N

10/ 562,112

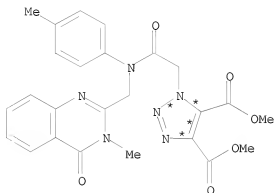


H



M

(5) \longrightarrow

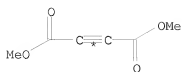


N

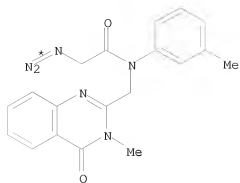
YIELD 79%

RX(5) RCT H 762-42-5, M 536697-62-8
 PRO N 1014987-16-6
 SOL 67-64-1 Me2CO
 CON 12 - 14 hours, reflux

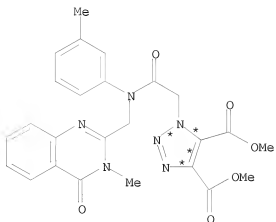
RX(6) OF 11 H + O ==> P



H



O

(6) \longrightarrow 

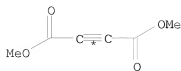
P

YIELD 77%

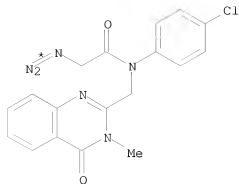
RX(6) RCT H 762-42-5, O 1014987-13-3
 PRO P 1014987-17-7
 SOL 67-64-1 Me2CO
 CON 12 - 14 hours, reflux

RX(7) OF 11 H + Q ==> R

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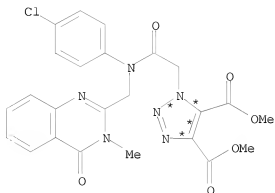


H



Q

(7) \longrightarrow

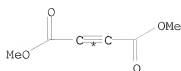


R

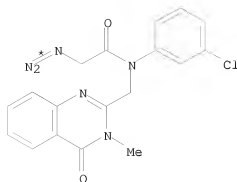
YIELD 69%

RX(7) RCT H 762-42-5, Q 536697-64-0
 PRO R 1014987-18-8
 SOL 67-64-1 Me2CO
 CON 12 - 14 hours, reflux

RX(8) OF 11 H + S ==> T

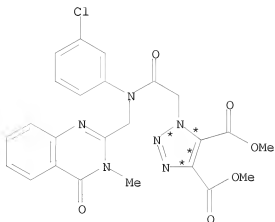


H



S

(8) →



T

YIELD 73%

RX(8) RCT H 762-42-5, S 1014987-14-4
 PRO T 1014987-19-9
 SOL 67-64-1 Me2CO
 CON 12 - 14 hours, reflux

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 148:355656 CASREACT

TITLE: Use of 2-(substituted vinyl)-4(3H)-quinazolinone and
 -4H-3,1-benzoxazinone in synthesis of heterocycles
 Morsy, J. M.

AUTHOR(S):
 CORPORATE SOURCE: Chemistry Department, Faculty of Education, Ain Shams
 University, Cairo, Egypt

SOURCE: Bulgarian Chemical Communications (2007), 39(2),

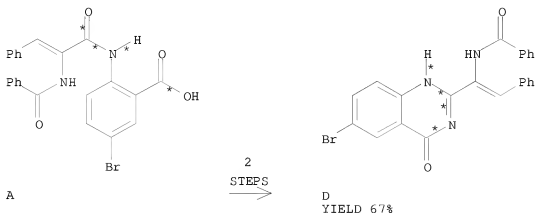
146-151
 CODEN: BCHCE4; ISSN: 0324-1130
 Bulgarian Academy of Sciences
 Journal
 English

PUBLISHER:
 DOCUMENT TYPE:
 LANGUAGE:
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 4H-3,1-Benzoxazinone I was transformed into 4(3H)-quinazolinones II (R = H, NH₂), which were converted to tetrazole III and thiazole IV in two-step processes. Tetrazole derivative V was also obtained from the starting benzoxazinone in a one-pot facile synthesis.

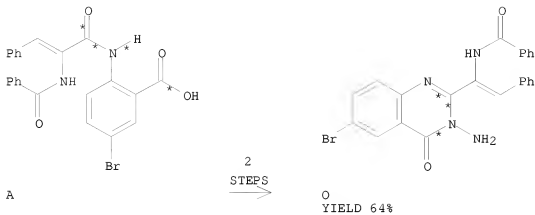
RX(18) OF 45 COMPOSED OF RX(1), RX(2)
 RX(18) A ==> D



RX(1) RCT A 1012086-13-3
 RGT C 108-24-7 Ac₂O
 PRO B 1012085-96-9
 SOL 108-24-7 Ac₂O
 CON 1 hour, 100 deg C

RX(2) RCT B 1012085-96-9
 RGT E 75-12-7 Formamide
 PRO D 1012085-97-0
 SOL 75-12-7 Formamide
 CON 3 hours, reflux
 NTE alternative reaction conditions shown

RX(19) OF 45 COMPOSED OF RX(1), RX(6)
 RX(19) A ==> O

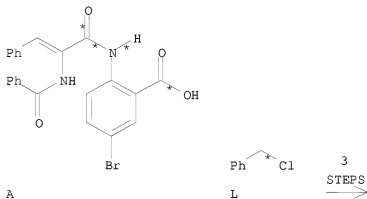


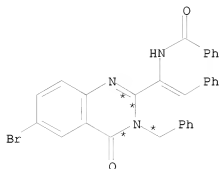
RX(1) RCT A 1012086-13-3
 RGT C 108-24-7 Ac2O
 PRO B 1012085-96-9
 SOL 108-24-7 Ac2O
 CON 1 hour, 100 deg C

RX(6) RCT B 1012085-96-9
 RGT P 7803-57-8 N2H4-H2O
 PRO O 1012086-01-9
 SOL 64-17-5 EtOH
 CON 3 hours, reflux

RX(35) OF 45 COMPOSED OF RX(1), RX(2), RX(5)

RX(35) A + L ==> M





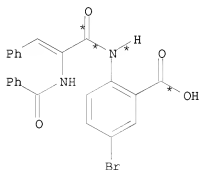
M
YIELD 62%

RX(1) RCT A 1012086-13-3
RGT C 108-24-7 Ac2O
PRO B 1012085-96-9
SOL 108-24-7 Ac2O
CON 1 hour, 100 deg C

RX(2) RCT B 1012085-96-9
RGT E 75-12-7 Formamide
PRO D 1012085-97-0
SOL 75-12-7 Formamide
CON 3 hours, reflux
NTE alternative reaction conditions shown

RX(5) RCT D 1012085-97-0, L 100-44-7
RGT N 110-86-1 Pyridine
PRO M 1012086-00-8
SOL 110-86-1 Pyridine
CON 3 hours, reflux

RX(36) OF 45 COMPOSED OF RX(1), RX(6), RX(7)
RX(36) A + R ==> S

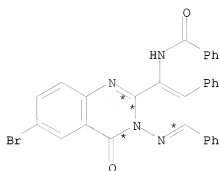


A



R

3
STEPS
→



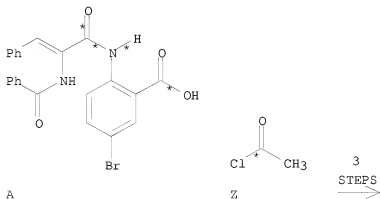
S
YIELD 55%

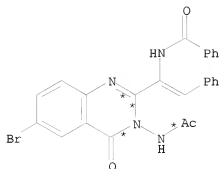
RX(1) RCT A 1012086-13-3
RGT C 108-24-7 Ac2O
PRO B 1012085-96-9
SOL 108-24-7 Ac2O
CON 1 hour, 100 deg C

RX(6) RCT B 1012085-96-9
RGT P 7803-57-8 N2H4-H2O
PRO O 1012086-01-9
SOL 64-17-5 EtOH
CON 3 hours, reflux

RX(7) RCT O 1012086-01-9, R 100-52-7
PRO S 1012086-02-0
CAT 110-89-4 Piperidine
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(37) OF 45 COMPOSED OF RX(1), RX(6), RX(10)
RX(37) A + Z ==> AA





AA

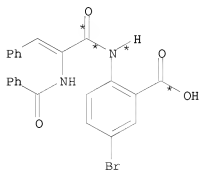
YIELD 72%

RX(1) RCT A 1012086-13-3
 RGT C 108-24-7 Ac2O
 PRO B 1012085-96-9
 SOL 108-24-7 Ac2O
 CON 1 hour, 100 deg C

 RX(6) RCT B 1012085-96-9
 RGT P 7803-57-8 N2H4-H2O
 PRO O 1012086-01-9
 SOL 64-17-5 EtOH
 CON 3 hours, reflux

 RX(10) RCT O 1012086-01-9, Z 75-36-5
 RGT N 110-86-1 Pyridine
 PRO AA 1012086-05-3
 SOL 110-86-1 Pyridine
 CON 3 hours, reflux

RX(38) OF 45 COMPOSED OF RX(1), RX(6), RX(11)
 RX(38) A + AB ==> AC

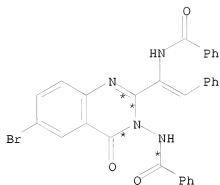


A



AB

3
 STEPS
 →



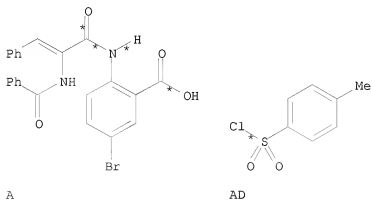
AC
YIELD 57%

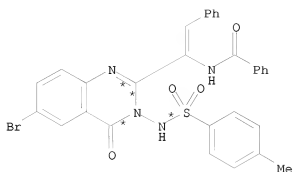
RX(1) RCT A 1012086-13-3
RGT C 108-24-7 Ac2O
PRO B 1012085-96-9
SOL 108-24-7 Ac2O
CON 1 hour, 100 deg C

RX(6) RCT B 1012085-96-9
RGT P 7803-57-8 N2H4-H2O
PRO O 1012086-01-9
SOL 64-17-5 EtOH
CON 3 hours, reflux

RX(11) RCT O 1012086-01-9, AB 98-88-4
RGT N 110-86-1 Pyridine
PRO AC 1012086-06-4
SOL 110-86-1 Pyridine
CON 3 hours, reflux

RX(39) OF 45 COMPOSED OF RX(1), RX(6), RX(12)
RX(39) A + AD ==> AE





AE

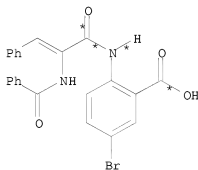
YIELD 50%

RX(1) RCT A 1012086-13-3
 RGT C 108-24-7 Ac2O
 PRO B 1012085-96-9
 SOL 108-24-7 Ac2O
 CON 1 hour, 100 deg C

RX(6) RCT B 1012085-96-9
 RGT P 7803-57-8 N2H4-H2O
 PRO O 1012086-01-9
 SOL 64-17-5 EtOH
 CON 3 hours, reflux

RX(12) RCT O 1012086-01-9, AD 98-59-9
 RGT N 110-86-1 Pyridine
 PRO AE 1012086-07-5
 SOL 110-86-1 Pyridine
 CON 4 hours, reflux

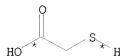
RX(44) OF 45 COMPOSED OF RX(1), RX(6), RX(7), RX(8)
 RX(44) A + R + U ==> V



A

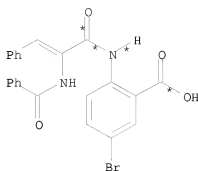


R



U

4
 STEPS
 →



A

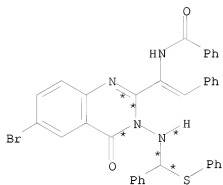


R



X

4
STEPS
→



Y

YIELD 57%

RX(1)	RCT	A 1012086-13-3
	RGT	C 108-24-7 Ac2O
	PRO	B 1012085-96-9
	SOL	108-24-7 Ac2O
	CON	1 hour, 100 deg C
RX(6)	RCT	B 1012085-96-9
	RGT	P 7803-57-8 N2H4-H2O
	PRO	O 1012086-01-9
	SOL	64-17-5 EtOH
	CON	3 hours, reflux
RX(7)	RCT	O 1012086-01-9, R 100-52-7
	PRO	S 1012086-02-0
	CAT	110-89-4 Piperidine
	SOL	64-17-5 EtOH
	CON	4 hours, reflux
RX(9)	RCT	S 1012086-02-0, X 108-98-5
	PRO	Y 1012086-04-2
	CAT	110-89-4 Piperidine
	SOL	71-43-2 Benzene

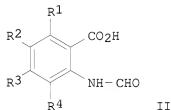
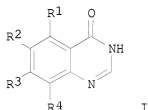
CON 2 hours, reflux

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 147:502385 CASREACT
 TITLE: Preparation of quinazolin-4-ones from
 N-formylanthranilic acids
 INVENTOR(S): Tanaka, Kazuo; Sato, Yoshifumi; Yoshimura, Takashi
 PATENT ASSIGNEE(S): Mitsubishi Gas Chemical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 9pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

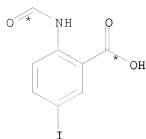
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2007290974	A	20071108	JP 2006-117729	20060421
PRIORITY APPLN. INFO.:			JP 2006-117729	20060421
OTHER SOURCE(S):		MARPAT 147:502385		

GI

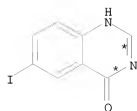


AB Quinazolin-4-ones I (R1-R4 = H, halo, NO2, C1-6 alkyl, alkoxy) are prepared by treatment of N-formylanthranilic acids II (R1-R4 = same as above) with HCONH2 and ammonia in the presence of AcOH and/or AcNH4 as catalyst. Thus, formylation of 5-iodoanthranilic acid with HCONH2 at 100° for 2 h gave 96.7% N-formyl-5-iodoanthranilic acid with 97.1% purity, which was autoclaved with HCONH2, AcNH4, and ammonia/MeOH at 150° for 2 h to afford 98.0% 6-iodoquinazolin-4-one.

RX(1) OF 4 A ==> B



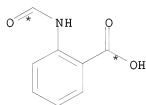
A



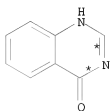
B
YIELD 98%

RX(1) RCT A 955998-77-3
RGT C 75-12-7 Formamide, D 7664-41-7 NH3, E 631-61-8 NH4OAc
PRO B 16064-08-7
SOL 7732-18-5 Water
CON 2 hours, 150 deg C

RX(2) OF 4 G ==> H



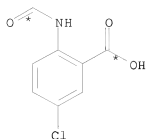
G



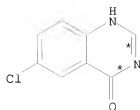
H
YIELD 98%

RX(2) RCT G 3342-77-6
RGT C 75-12-7 Formamide, D 7664-41-7 NH3, I 64-19-7 AcOH
PRO H 491-36-1
SOL 7732-18-5 Water
CON 2 hours, 150 deg C

RX(3) OF 4 J ==> K



J

K
YIELD 96%

RX(3) RCT J 26208-56-0
 RGT C 75-12-7 Formamide, D 7664-41-7 NH3, I 64-19-7 AcOH
 PRO K 16064-14-5
 SOL 7732-18-5 Water
 CON 2 hours, 150 deg C

L3 ANSWER 9 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 147:486453 CASREACT
 TITLE: Quinazolin-4-one derivatives as B-Raf inhibitors,
 process for their preparation and pharmaceutical
 compositions containing them for treating cancer
 INVENTOR(S): Aquila, Brian; Lyne, Paul; Pontz, Timothy
 PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca Uk Limited
 SOURCE: PCI Int. Appl., 52pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

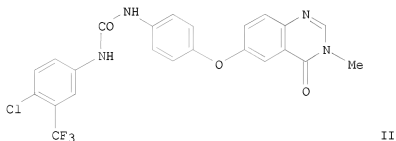
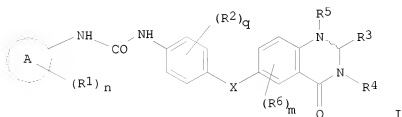
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007119055	A1	20071025	WO 2007-GB1389	20070417
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM EP 2010504 A1 20090107 EP 2007-732431 20070417 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS				

PRIORITY APPLN. INFO.:

US 2006-745038P 20060418

OTHER SOURCE(S):
GI

MARPAT 147:486453

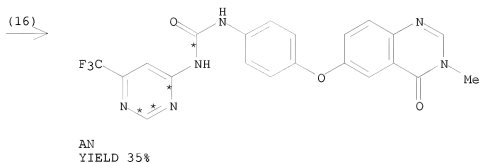
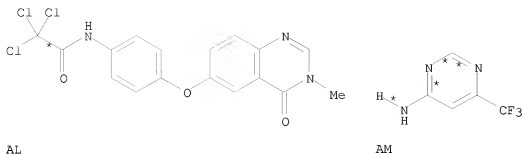


AB The invention relates to chemical compds. of the formula I (wherein Ring A is carbocyclyl or heterocyclyl; R1 is a substituent on C and is halo, nitro, etc.; n is 0-4; R2 is halo, nitro, cyano, OH, etc.; q is 0-2; X is NR16 or O; R3 and R6 are H, halo, nitro, cyano, etc.; R4, R5 and R16 are H, Cl-6alkyl, Cl-6alkanoyl, etc.; m is 3 wherein the value of R6 may be the same or different) or pharmaceutically acceptable salts thereof, which possess B-Raf inhibitory activity and are accordingly useful for their anti-cancer activity and thus in methods of treatment of the human or animal body. The invention also relates to processes for the manufacture of said chemical compds., to pharmaceutical compns. containing them and to their

use in the manufacture of medicaments of use in the production of an anti-cancer effect

in a warm-blooded animal such as man. Example compound II was prepared by reacting 1-chloro-4-isocyanato-2-(trifluoromethyl)benzene and 6-(4-aminophenoxy)-3-methylquinazolin-4(3H)-one. In the B-Raf in vitro AlphaScreen assay, II had an IC50 of 0.287 μ M.

RX(16) OF 215 ...AL + AM ==> AN



RX(16) RCT AL 953414-07-8, AM 672-41-3

STAGE(1)

RGT AO 1310-73-2 NaOH

SOL 67-68-5 DMSO

CON SUBSTAGE(1) 80 deg C

SUBSTAGE(2) 80 deg C -> 25 deg C

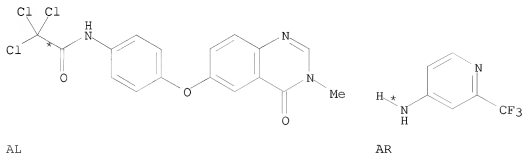
STAGE(2)

RGT AP 7732-18-5 Water

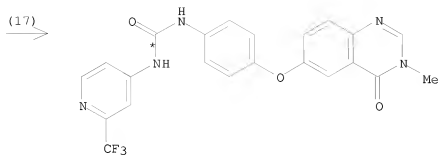
CON 25 deg C

PRO AN 953414-03-4

RX(17) OF 215 ...AL + AR ==> AS



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AS

RX(17) RCT AL 953414-07-8, AR 147149-98-2

STAGE(1)

RGT AO 1310-73-2 NaOH

SOL 67-68-5 DMSO

CON SUBSTAGE(1) 80 deg C

SUBSTAGE(2) 80 deg C -> 25 deg C

STAGE(2)

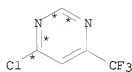
RGT AP 7732-18-5 Water

CON 25 deg C

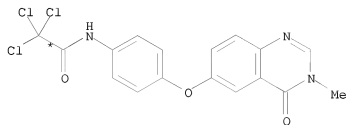
PRO AS 953414-04-5

RX(66) OF 215 COMPOSED OF RX(23), RX(16)

RX(66) BH + AL ==> AN



BH



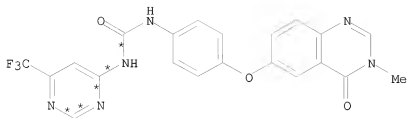
AL

2

STEPS



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AN
YIELD 35%

RX(23) RCT BH 37552-81-1
RGT BI 7664-41-7 NH3
PRO AM 672-41-3
SOL 67-56-1 MeOH
CON 12 hours, 25 deg C
NTE overall yield is 29% over two steps

RX(16) RCT AL 953414-07-8, AM 672-41-3

STAGE(1)

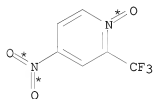
RGT AO 1310-73-2 NaOH
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 80 deg C
SUBSTAGE(2) 80 deg C -> 25 deg C

STAGE(2)

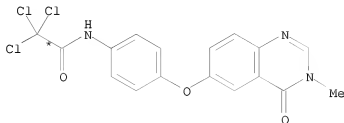
RGT AP 7732-18-5 Water
CON 25 deg C

PRO AN 953414-03-4

RX(90) OF 215 COMPOSED OF RX(43), RX(17)
RX(90) CM + AL ==> AS



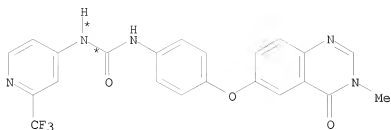
CM



AL

2
STEPS
→

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AS

RX(43) RCT CM 147149-97-1
RGT AU 1333-74-0 H2
PRO AR 147149-98-2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 12 hours, room temperature
NTE overall yield is 9% over two steps

RX(17) RCT AL 953414-07-8, AR 147149-98-2

STAGE(1)

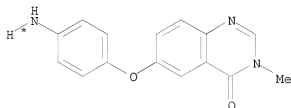
RGT AO 1310-73-2 NaOH
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 80 deg C
SUBSTAGE(2) 80 deg C -> 25 deg C

STAGE(2)

RGT AP 7732-18-5 Water
CON 25 deg C

PRO AS 953414-04-5

RX(115) OF 215 COMPOSED OF REACTION SEQUENCE RX(22), RX(16)
AND REACTION SEQUENCE RX(50), RX(23), RX(16)
...B + BF ==> AL...
...DE + AL ==> AN

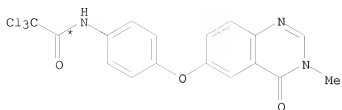


B



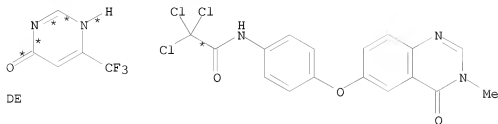
BF

3
STEPS
→

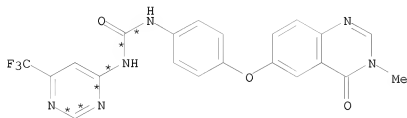


AL

START NEXT REACTION SEQUENCE



AL

3
STEPS
→

AN

YIELD 35%

RX(22) RCT B 953414-05-6, BF 76-03-9

STAGE(1)

RGT BG 7719-12-2 PC13

CON reflux

STAGE(2)

RGT AP 7732-18-5 Water

CON cooled

PRO AL 953414-07-8

RX(50)

RCT DE 1546-78-7

RGT DF 824-72-6 PhP(O)Cl2

PRO BH 37552-81-1

CON SUBSTAGE(1) 30 minutes, 130 deg C

SUBSTAGE(2) 130 deg C -> 25 deg C

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RX(23) RCT BH 37552-81-1
RGT BI 7664-41-7 NH3
PRO AM 672-41-3
SOL 67-56-1 MeOH
CON 12 hours, 25 deg C
NTE overall yield is 29% over two steps

RX(16) RCT AL 953414-07-8, AM 672-41-3

STAGE(1)

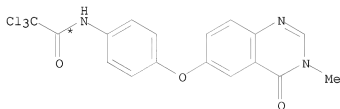
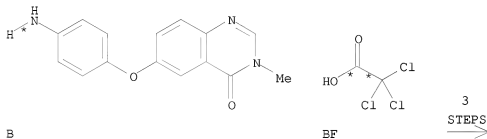
RGT AO 1310-73-2 NaOH
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 80 deg C
SUBSTAGE(2) 80 deg C -> 25 deg C

STAGE(2)

RGT AP 7732-18-5 Water
CON 25 deg C

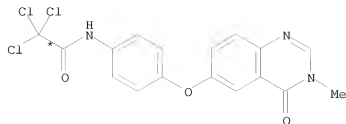
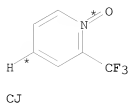
PRO AN 953414-03-4

RX(168) OF 215 COMPOSED OF REACTION SEQUENCE RX(22), RX(17)
AND REACTION SEQUENCE RX(44), RX(43), RX(17)
...B + BF ==> AL...
...CJ + AL ==> AS

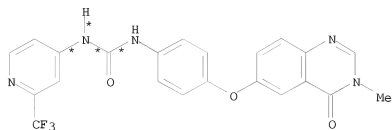


AL

START NEXT REACTION SEQUENCE



3
STEPS
→



RX(22) RCT B 953414-05-6, BF 76-03-9

STAGE(1)

RGT BG 7719-12-2 PC13
CON reflux

STAGE(2)

RGT AP 7732-18-5 Water
CON cooled

PRO AL 953414-07-8

RX(44) RCT CJ 22253-71-0

STAGE(1)

RGT CN 7664-93-9 H2SO4, CO 7697-37-2 HNO3
SOL 7732-18-5 Water
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 4 hours, 125 deg C

STAGE(2)

RGT AP 7732-18-5 Water
CON cooled

STAGE(3)

RGT AO 1310-73-2 NaOH
SOL 7732-18-5 Water
CON pH 7

PRO CM 147149-97-1

NTE regioselective, fuming nitric acid

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RX(43) RCT CM 147149-97-1
RGT AU 1333-74-0 H2
PRO AR 147149-98-2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 12 hours, room temperature
NTE overall yield is 9% over two steps

RX(17) RCT AL 953414-07-8, AR 147149-98-2

STAGE(1)

RGT AO 1310-73-2 NaOH
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 80 deg C
SUBSTAGE(2) 80 deg C -> 25 deg C

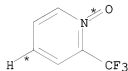
STAGE(2)

RGT AP 7732-18-5 Water
CON 25 deg C

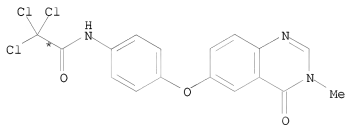
PRO AS 953414-04-5

RX(169) OF 215 COMPOSED OF RX(44), RX(43), RX(17)

RX(169) CJ + AL ==> AS

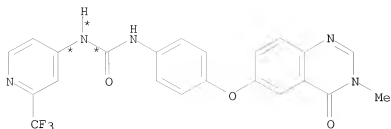


CJ



AL

3
STEPS
→



AS

RX(44) RCT CJ 22253-71-0

STAGE(1)

RGT CN 7664-93-9 H_2SO_4 , CO 7697-37-2 HNO_3

SOL 7732-18-5 Water

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 4 hours, 125 deg C

STAGE(2)

RGT AP 7732-18-5 Water

CON cooled

STAGE(3)

RGT AO 1310-73-2 NaOH

SOL 7732-18-5 Water

CON pH 7

PRO CM 147149-97-1

NTE regioselective, fuming nitric acid

RX(43)

RCT CM 147149-97-1

RGT AU 1333-74-0 H_2

PRO AR 147149-98-2

CAT 7440-05-3 Pd

SOL 67-56-1 MeOH

CON 12 hours, room temperature

NTE overall yield is 9% over two steps

RX(17)

RCT AL 953414-07-8, AR 147149-98-2

STAGE(1)

RGT AO 1310-73-2 NaOH

SOL 67-68-5 DMSO

CON SUBSTAGE(1) 80 deg C

SUBSTAGE(2) 80 deg C \rightarrow 25 deg C

STAGE(2)

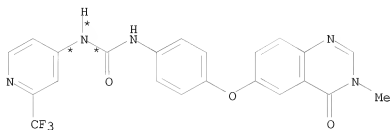
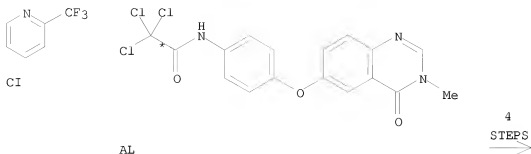
RGT AP 7732-18-5 Water

CON 25 deg C

PRO AS 953414-04-5

RX(170) OF 215 COMPOSED OF RX(42), RX(44), RX(43), RX(17)

RX(170) CI + AL \Rightarrow AS



AS

RX(42) RCT CI 368-48-9

STAGE(1)

RGT CK 937-14-4 MCPBA
 SOL 75-09-2 CH₂Cl₂
 CON 12 hours, 25 deg C

STAGE(2)

RGT CL 144-55-8 NaHCO₃
 SOL 7732-18-5 Water

PRO CJ 22253-71-0

RX(44) RCT CJ 22253-71-0

STAGE(1)

RGT CN 7664-93-9 H₂SO₄, CO 7697-37-2 HNO₃
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 4 hours, 125 deg C

STAGE(2)

RGT AP 7732-18-5 Water
 CON cooled

STAGE(3)

RGT AO 1310-73-2 NaOH
 SOL 7732-18-5 Water
 CON pH 7

PRO CM 147149-97-1
 NTE regioselective, fuming nitric acid

RX(43) RCT CM 147149-97-1
 RGT AU 1333-74-0 H2
 PRO AR 147149-98-2
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 CON 12 hours, room temperature
 NTE overall yield is 9% over two steps

RX(17) RCT AL 953414-07-8, AR 147149-98-2

STAGE(1)

RGT AO 1310-73-2 NaOH
 SOL 67-68-5 DMSO
 CON SUBSTAGE(1) 80 deg C
 SUBSTAGE(2) 80 deg C -> 25 deg C

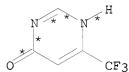
STAGE(2)

RGT AP 7732-18-5 Water
 CON 25 deg C

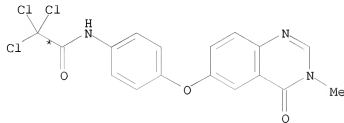
PRO AS 953414-04-5

RX(176) OF 215 COMPOSED OF RX(50), RX(23), RX(16)

RX(176) DE + AL ==> AN

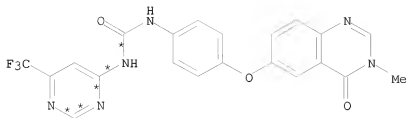


DE



AL

3
 STEPS
 →



AN
YIELD 35%

RX(50) RCT DE 1546-78-7
RGT DF 824-72-6 PhP(O)Cl2
PRO BH 37552-81-1
CON SUBSTAGE(1) 30 minutes, 130 deg C
SUBSTAGE(2) 130 deg C -> 25 deg C

RX(23) RCT BH 37552-81-1
RGT BI 7664-41-7 NH3
PRO AM 672-41-3
SOL 67-56-1 MeOH
CON 12 hours, 25 deg C
NTE overall yield is 29% over two steps

RX(16) RCT AL 953414-07-8, AM 672-41-3

STAGE(1)
RGT AO 1310-73-2 NaOH
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 80 deg C
SUBSTAGE(2) 80 deg C -> 25 deg C

STAGE(2)
RGT AP 7732-18-5 Water
CON 25 deg C

PRO AN 953414-03-4

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 147:448747 CASREACT
TITLE: Synthesis, insecticidal and antimicrobial activities of some heterocyclic derivatives of quinazolinone
AUTHOR(S): Singh, Tripti; Sharma, Shalabh; Srivastava, Virendra Kishore; Kumar, Ashok
CORPORATE SOURCE: Medicinal Chemistry Division, Department of Pharmacology, Lala Lajpat Rai Memorial Medical College, Meerut, 250 004, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2006), 45B(11), 2558-2565

PUBLISHER:

CODEN: IJSBDB; ISSN: 0376-4699

National Institute of Science Communication and
Information Resources

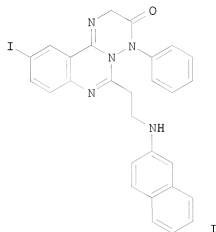
DOCUMENT TYPE:

Journal

LANGUAGE:

English

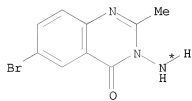
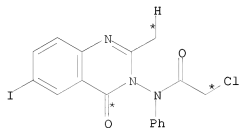
GI



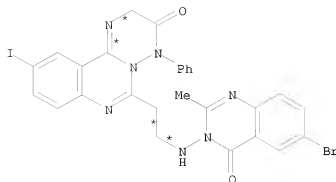
AB Some triazinoquinazoline derivs., e.g., I, have been synthesized from 4-phenyl-2,3-dihydro-6-methyl-10-iodo[1,2,3]-triazino[2,3-c]quinazolin-5-one by introducing aromatic nuclei via Mannich reaction with arylamines. These compds. were screened for insecticidal, anti-fungal and antibacterial activities. Compound I was found to be the most potent compound compared with the standard. Moreover, compound I also showed antibacterial activity. The structures of these compds. were elucidated by IR, ¹H NMR, mass spectroscopy and elemental anal.

RX(22) OF 69 COMPOSED OF RX(5), RX(9)

RX(22) M + X + R ==> Y



2
STEPS
→



Y
YIELD 45%

RX(5) RCT M 952430-81-8
RGT P 631-61-8 NH4OAc
PRO O 952430-82-9
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 8 hours, reflux

RX(9) RCT O 952430-82-9, X 71822-97-4, R 50-00-0
RGT K 64-17-5 EtOH
PRO Y 952430-85-2
CON 8 hours, reflux
NTE Mannich reaction

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 147:448727 CASREACT

TITLE: Synthesis of 2-methyl-3-tolyl-4-quinazolinone hydrochloride

AUTHOR(S): Zeng, Guiping; Sun, Fuqiang

CORPORATE SOURCE: College of Pharmaceutical Science, Guangdong College

of Pharmacy, Guangzhou, 510224, Peop. Rep. China

SOURCE: Huaxue Shijie (2005), 46(12), 732-733, 725

CODEN: HUAKAB; ISSN: 0367-6358

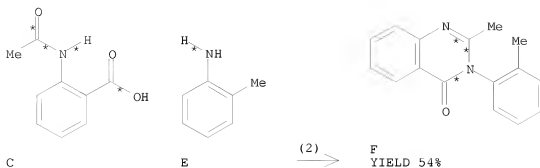
PUBLISHER: Shanghaiishi Huaxue Huagong Xuehui

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

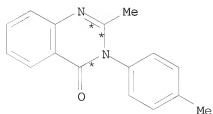
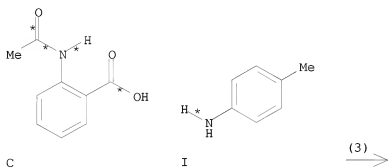
AB ;2-Methyl-3-(methylphenyl)-4-quinazolinone hydrochloride was prepared from anthranilic acid by condensation with acetic anhydride, cyclization with o-methylaniline or p-methylaniline in the presence of a dehydration agent (POCl₃, H₂SO₄, P₂O₅) and salt formation with HCl. The compds. thus prepared included methaqualone hydrochloride [i.e., 2-methyl-3-(2-methylphenyl)-4(3H)-quinazolinone hydrochloride] and 2-methyl-3-(4-methylphenyl)-4(3H)-quinazolinone hydrochloride.

RX(2) OF 9 ...C + E ==> F



RX(2) RCT C 89-52-1, E 95-53-4
 RGT G 10025-87-3 POC13
 PRO F 72-44-6
 SOL 108-88-3 PhMe
 CON 1.5 hours, reflux
 NTE optimization study, optimized on reaction time

RX(3) OF 9 ...C + I ==> J

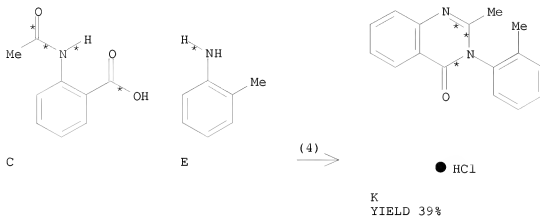


J
YIELD 40%

RX(3) RCT C 89-52-1, I 106-49-0
 RGT G 10025-87-3 POC13
 PRO J 22316-59-2
 SOL 108-88-3 PhMe

CON 1.5 hours, reflux
 NTE optimization study, optimized on reaction time

RX(4) OF 9 ...C + E ==> K



RX(4) RCT C 89-52-1, E 95-53-4

STAGE(1)

RGT G 10025-87-3 POC13

SOL 108-88-3 PhMe

CON 1.5 hours, reflux

STAGE(2)

RGT L 7647-01-0 HCl

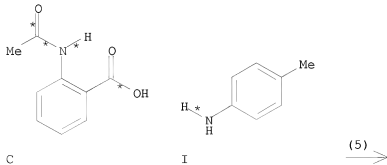
SOL 7732-18-5 Water

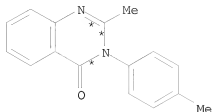
CON heated

PRO K 340-56-7

NTE optimization study, optimized on reagent

RX(5) OF 9 ...C + I ==> M





● HCl

M
YIELD 56%

RX(5) RCT C 89-52-1, I 106-49-0

STAGE(1)

RGT G 10025-87-3 POC13
SOL 108-88-3 PhMe
CON 1.5 hours, reflux

STAGE(2)

RGT L 7647-01-0 HCl
SOL 7732-18-5 Water
CON heated

PRO M 80257-03-0
NTE optimization study, optimized on reagent

L3 ANSWER 12 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 147:406780 CASREACT

TITLE: Synthesis of 7-bromo-6-chloro-4-quinazolinone and
5-bromo-6-chloro-4-quinazolinone

AUTHOR(S): Zhang, Yue; Niu, Yuhuan; Dong, Bofang; Wang, Yinhua;
Di, Xiaotao; Du, Huiru

CORPORATE SOURCE: Chemical and Pharmaceutical Engineering College, Hebei
University of Science and Technology, Shijiazhuang,
Hebei Province, 050018, Peop. Rep. China

SOURCE: Jingxi Huagong (2006), 23(8), 822-824
CODEN: JIHUFJ; ISSN: 1003-5214

PUBLISHER: Jingxi Huagong Bianjibu

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

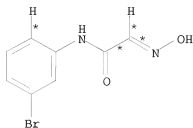
AB N-(3-Bromophenyl)-2-(hydroxyimino)acetamide was synthesized from
m-bromoaniline and chloral hydrate in 90.5% yield. By treatment with
concentrated sulfuric acid this compound cyclized to give a mixture of
6-bromoisatin

and 4-bromoisatin in 97.6% yield. Chlorination of bromoisatin gave
6-bromo-5-chloroisatin in 86.8% yield and acetic acid was used as solvent
instead of toxic nitrobenzene. The latter compound was oxidized by aqueous
hydrogen peroxide to form 2-amino-4-bromo-5-chlorobenzoic acid. Treatment

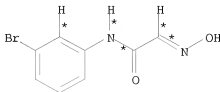
with phosphorous oxychloride and formamide gave
 7-bromo-6-chloro-4(3H)-quinazolinone. The total yield was 12.14%.
 5-Bromo-6-chloro-4(3H)-quinazolinone was synthesized in the same way and
 the total yield was 13.47%.

RX(26) OF 28 COMPOSED OF RX(2), RX(7), RX(8), RX(9)

RX(26) 2 C + R ==> W



C

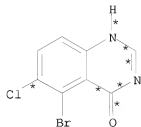


C



R

4
 STEPS
 →



W
 YIELD 65%

RX(2) RCT C 65971-74-6

STAGE(1)

RGT E 7664-93-9 H2SO4

SOL 7732-18-5 Water

CON SUBSTAGE(1) room temperature -> 50 deg C

SUBSTAGE(2) 50 deg C

SUBSTAGE(3) 0.5 hours, 70 - 75 deg C

SUBSTAGE(4) 75 deg C -> room temperature

STAGE(2)

RGT G 7732-18-5 Water

CON 0.5 hours, cooled

STAGE(3)

RGT J 1310-73-2 NaOH

SOL 7732-18-5 Water
CON room temperature

STAGE(4)

RGT E 7664-93-9 H2SO4
SOL 7732-18-5 Water
CON room temperature, pH 8

STAGE(5)

RGT K 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, pH 3.5

PRO H 6326-79-0, I 20780-72-7

RX(7)

RCT I 20780-72-7
RGT O 64-19-7 AcOH, M 7719-09-7 SOCl2, N 7791-25-5 SO2Cl2
PRO U 65971-75-7
CON SUBSTAGE(1) room temperature -> 80 deg C
SUBSTAGE(2) 80 - 85 deg C
SUBSTAGE(3) 85 deg C -> 90 deg C
SUBSTAGE(4) 45 minutes, 85 - 95 deg C
SUBSTAGE(5) 95 deg C -> room temperature
NTE catalyst used

RX(8)

RCT U 65971-75-7

STAGE(1)

RGT J 1310-73-2 NaOH, Q 7722-84-1 H2O2
SOL 7732-18-5 Water
CON SUBSTAGE(1) 20 minutes, room temperature
SUBSTAGE(2) 45 minutes, room temperature

STAGE(2)

RGT K 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, acidify

PRO V 65971-76-8

RX(9)

RCT R 75-12-7, V 65971-76-8

STAGE(1)

RGT T 10025-87-3 POC13
CON SUBSTAGE(1) room temperature -> 90 deg C
SUBSTAGE(2) 90 - 95 deg C
SUBSTAGE(3) 30 minutes, 90 - 95 deg C
SUBSTAGE(4) cooled

STAGE(2)

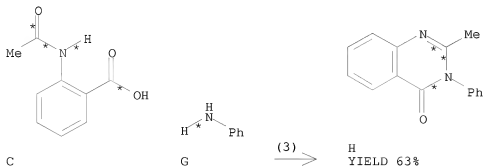
RGT G 7732-18-5 Water
CON cooled

PRO W 65971-77-9

NTE 13% overall yield from 3-bromo-Benzenamine

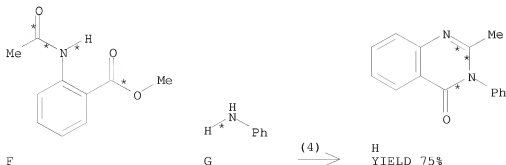
L3 ANSWER 13 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 147:344042 CASREACT
 TITLE: Synthesis of new 4(3H)-quinazolinone derivatives
 AUTHOR(S): Truong, The Ky; Nguyen, Anh Tuan; Ly, Da Thoi; Pham, Khanh Phong Lan
 CORPORATE SOURCE: Dept. Pharmacy, Ho Chi Minh City College of Pharmacy and Medicine, Vietnam
 SOURCE: Tap Chi Hoa Hoc (2006), 44(4), 445-448
 CODEN: TCHHDC; ISSN: 0378-2336
 PUBLISHER: Toa Soan Tap Chi Hoa Hoc
 DOCUMENT TYPE: Journal
 LANGUAGE: Vietnamese
 AB For the pharmacomodulation of 4(3H)-quinazolinone, a heterocycle with many advantages in therapy, the authors implemented nucleophilic substitution on the chloromethyl group of position 2 using phenol and amine derivs. to give new compds. that showed potential antifungal and antibacterial activities. One antibacterial and antifungal triazolymethylquinazolinone derivative synthesized in this research project showed MIC of 16 µg/mL against *Candida albicans*.

RX(3) OF 70 ...C + G ==> H...



RX(3) RCT C 89-52-1, G 62-53-3
 PRO H 2385-23-1
 NTE alternative preparation shown

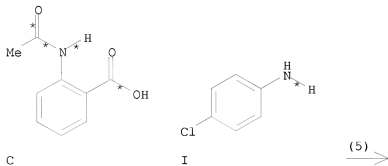
RX(4) OF 70 ...F + G ==> H...



10/ 562,112

RX(4) RCT F 2719-08-6, G 62-53-3
PRO H 2385-23-1
NTE alternative preparation shown

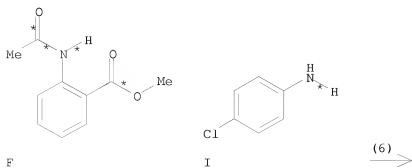
RX(5) OF 70 ...C + I ==> J...

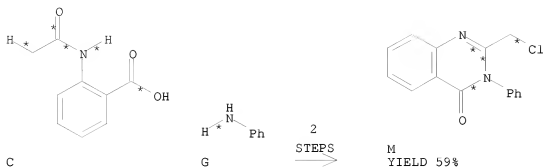


J
YIELD 74%

RX(5) RCT C 89-52-1, I 106-47-8
PRO J 1788-93-8
NTE alternative preparation shown

RX(6) OF 70 ...F + I ==> J...

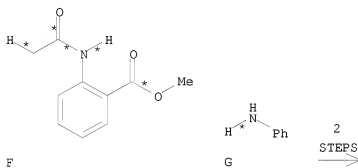




RX(3) RCT C 89-52-1, G 62-53-3
 PRO H 2385-23-1
 NTE alternative preparation shown

RX(8) RCT H 2385-23-1
 RGT N 128-08-5 Bromosuccinimide
 PRO M 22312-77-2
 CAT 110-86-1 Pyridine
 SOL 67-66-3 CHCl₃

RX(24) OF 70 COMPOSED OF RX(4), RX(8)
 RX(24) F + G ==> M



RX(4) RCT F 2719-08-6, G 62-53-3

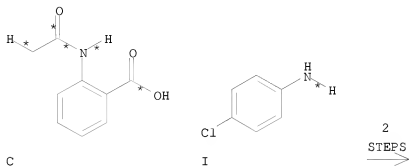
10/ 562,112

PRO H 2385-23-1
NTE alternative preparation shown

RX(8) RCT H 2385-23-1
RGT N 128-08-5 Bromosuccinimide
PRO M 22312-77-2
CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl₃

RX(25) OF 70 COMPOSED OF RX(5), RX(9)

RX(25) C + I ==> Q



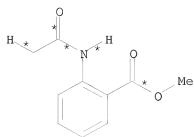
Q
YIELD 53%

RX(5) RCT C 89-52-1, I 106-47-8
PRO J 1788-93-8
NTE alternative preparation shown

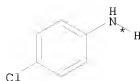
RX(9) RCT J 1788-93-8
RGT N 128-08-5 Bromosuccinimide
PRO Q 22280-87-1
CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl₃

RX(26) OF 70 COMPOSED OF RX(6), RX(9)

RX(26) F + I ==> Q

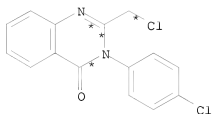


F



I

2
STEPS
→



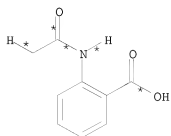
Q

YIELD 53%

RX(6) RCT F 2719-08-6, I 106-47-8
PRO J 1788-93-8
NIE alternative preparation shown

RX(9) RCT J 1788-93-8
RGT N 128-08-5 Bromosuccinimide
PRO Q 22280-87-1
CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl₃

RX(39) OF 70 COMPOSED OF RX(3), RX(8), RX(10)
RX(39) C + G + R ==> S



C

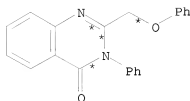


G



R

3
STEPS
→



S

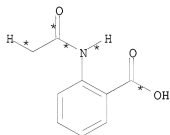
YIELD 39%

RX(3) RCT C 89-52-1, G 62-53-3
 PRO H 2385-23-1
 NTE alternative preparation shown

RX(8) RCT H 2385-23-1
 RGT N 128-08-5 Bromosuccinimide
 PRO M 22312-77-2
 CAT 110-86-1 Pyridine
 SOL 67-66-3 CHCl₃

RX(10) RCT M 22312-77-2, R 108-95-2
 RGT T 1310-73-2 NaOH
 PRO S 20873-22-7
 SOL 68-12-2 DMF
 NTE Williamson reaction

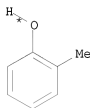
RX(40) OF 70 COMPOSED OF RX(3), RX(8), RX(11)
 RX(40) C + G + V ==> W



C

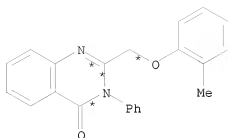


G



V

3
 STEPS
 ==>



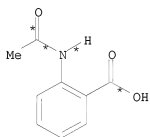
W
YIELD 23%

RX(3) RCT C 89-52-1, G 62-53-3
PRO H 2385-23-1
NTE alternative preparation shown

RX(8) RCT H 2385-23-1
RGT N 128-08-5 Bromosuccinimide
PRO M 22312-77-2
CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl₃

RX(11) RCT M 22312-77-2, V 95-48-7
RGT T 1310-73-2 NaOH
PRO W 948312-75-2
SOL 68-12-2 DMF
NTE Williamson reaction

RX(41) OF 70 COMPOSED OF RX(3), RX(8), RX(12)
RX(41) C + G + V ==> X



C

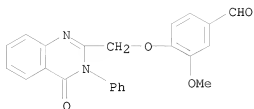


G



V

3
STEPS
➞



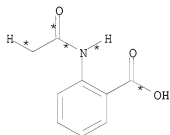
X
YIELD 22%

RX(3) RCT C 89-52-1, G 62-53-3
PRO H 2385-23-1
NTE alternative preparation shown

RX(8) RCT H 2385-23-1
RGT N 128-08-5 Bromosuccinimide
PRO M 22312-77-2
CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl₃

RX(12) RCT M 22312-77-2, V 95-48-7
RGT T 1310-73-2 NaOH
PRO X 948312-76-3
SOL 68-12-2 DMF
NTE Williamson reaction, an unspecified acetal of vanillin used

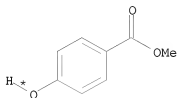
RX(42) OF 70 COMPOSED OF RX(3), RX(8), RX(13)
RX(42) C + G + Y ==> Z



C

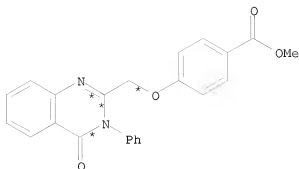


G



Y

3
STEPS
→



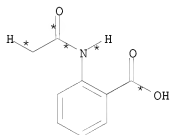
Z
YIELD 33%

RX(3) RCT C 89-52-1, G 62-53-3
PRO H 2385-23-1
NTE alternative preparation shown

RX(8) RCT H 2385-23-1
RGT N 128-08-5 Bromosuccinimide
PRO M 22312-77-2
CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl₃

RX(13) RCT M 22312-77-2, Y 99-76-3
RGT T 1310-73-2 NaOH
PRO Z 948312-77-4
SOL 68-12-2 DMF
NTE Williamson reaction

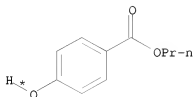
RX(43) OF 70 COMPOSED OF RX(3), RX(8), RX(14)
RX(43) C + G + AA ==> AB



C

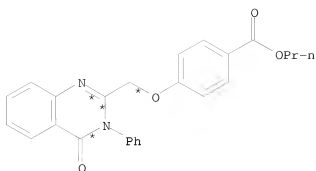


G



AA

3
STEPS
→



AB

YIELD 29%

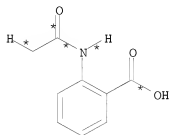
RX(3) RCT C 89-52-1, G 62-53-3
 PRO H 2385-23-1
 NTE alternative preparation shown

RX(8) RCT H 2385-23-1
 RGT N 128-08-5 Bromosuccinimide
 PRO M 22312-77-2
 CAT 110-86-1 Pyridine
 SOL 67-66-3 CHCl₃

RX(14) RCT M 22312-77-2, AA 94-13-3
 RGT T 1310-73-2 NaOH
 PRO AB 948312-78-5
 SOL 68-12-2 DMF
 NTE Williamson reaction

RX(44) OF 70 COMPOSED OF RX(3), RX(8), RX(15)

RX(44) C + G + AC ==> AD



C

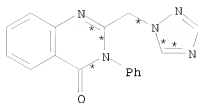


G



AC

3
 STEPS
 →



AD
YIELD 31%

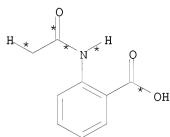
RX(3) RCT C 89-52-1, G 62-53-3
PRO H 2385-23-1
NTE alternative preparation shown

RX(8) RCT H 2385-23-1
RGT N 128-08-5 Bromosuccinimide
PRO M 22312-77-2
CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl₃

RX(15) RCT M 22312-77-2, AC 288-88-0
PRO AD 948312-72-9
CAT 7440-23-5 Na
SOL 67-56-1 MeOH

RX(45) OF 70 COMPOSED OF RX(3), RX(8), RX(16)

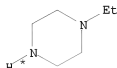
RX(45) C + G + AG ==> AH



C

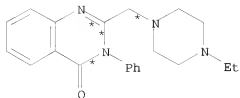


G



AG

3
STEPS
=>



AH
YIELD 24%

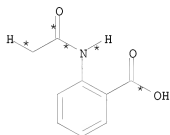
10/ 562,112

RX(3) RCT C 89-52-1, G 62-53-3
 PRO H 2385-23-1
 NTE alternative preparation shown

RX(8) RCT H 2385-23-1
 RGT N 128-08-5 Bromosuccinimide
 PRO M 22312-77-2
 CAT 110-86-1 Pyridine
 SOL 67-66-3 CHCl3

RX(16) RCT M 22312-77-2, AG 5308-25-8
 PRO AH 948312-73-0
 CAT 7440-23-5 Na
 SOL 67-56-1 MeOH

RX(46) OF 70 COMPOSED OF RX(3), RX(8), RX(17)
 RX(46) C + G + AI ==> AJ



C

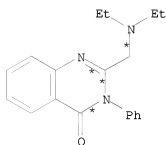


G



AI

3
 STEPS
 →



AJ
 YIELD 40%

RX(3) RCT C 89-52-1, G 62-53-3
 PRO H 2385-23-1
 NTE alternative preparation shown

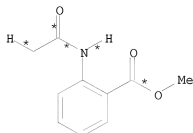
RX(8) RCT H 2385-23-1
 RGT N 128-08-5 Bromosuccinimide
 PRO M 22312-77-2

10/ 562,112

CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl₃

RX(17) RCT M 22312-77-2, AI 109-89-7
PRO AJ 948312-74-1
CAT 7440-23-5 Na
SOL 67-56-1 MeOH

RX(47) OF 70 COMPOSED OF RX(4), RX(8), RX(10)
RX(47) F + G + R ==> S



F

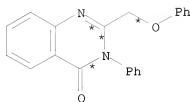


G



R

3
STEPS
→



S

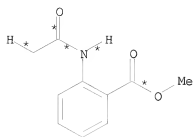
YIELD 39%

RX(4) RCT F 2719-08-6, G 62-53-3
PRO H 2385-23-1
NTE alternative preparation shown

RX(8) RCT H 2385-23-1
RGT N 128-08-5 Bromosuccinimide
PRO M 22312-77-2
CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl₃

RX(10) RCT M 22312-77-2, R 108-95-2
RGT T 1310-73-2 NaOH
PRO S 20873-22-7
SOL 68-12-2 DMF
NTE Williamson reaction

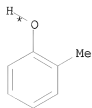
RX(48) OF 70 COMPOSED OF RX(4), RX(8), RX(11)
RX(48) F + G + V ==> W



F

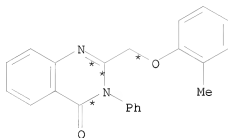


G



V

3
STEPS
→



W

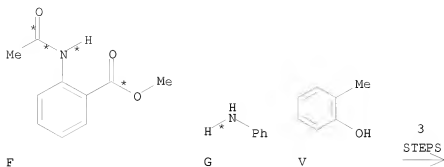
YIELD 23%

RX(4) RCT F 2719-08-6, G 62-53-3
PRO H 2385-23-1
NTE alternative preparation shown

RX(8) RCT H 2385-23-1
RGT N 128-08-5 Bromosuccinimide
PRO M 22312-77-2
CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl3

RX(11) RCT M 22312-77-2, V 95-48-7
RGT T 1310-73-2 NaOH
PRO W 948312-75-2
SOL 68-12-2 DMF
NTE Williamson reaction

RX(49) OF 70 COMPOSED OF RX(4), RX(8), RX(12)
RX(49) F + G + V ==> X



X
YIELD 22%

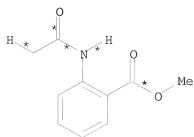
RX(4) RCT F 2719-08-6, G 62-53-3
 PRO H 2385-23-1
 NTE alternative preparation shown

RX(8) RCT H 2385-23-1
 RGT N 128-08-5 Bromosuccinimide
 PRO M 22312-77-2
 CAT 110-86-1 Pyridine
 SOL 67-66-3 CHCl₃

RX(12) RCT M 22312-77-2, V 95-48-7
 RGT T 1310-73-2 NaOH
 PRO X 948312-76-3
 SOL 68-12-2 DMF
 NTE Williamson reaction, an unspecified acetal of vanillin used

RX(50) OF 70 COMPOSED OF RX(4), RX(8), RX(13)

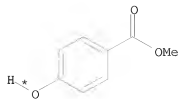
RX(50) F + G + Y ==> Z



F

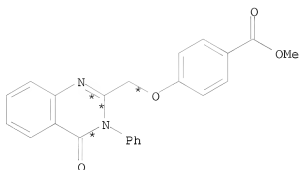


G



Y

3
STEPS
→



Z

YIELD 33%

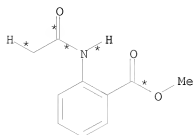
RX(4) RCT F 2719-08-6, G 62-53-3
PRO H 2385-23-1
NTE alternative preparation shown

RX(8) RCT H 2385-23-1
RGT N 128-08-5 Bromosuccinimide
PRO M 22312-77-2
CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl3

RX(13) RCT M 22312-77-2, Y 99-76-3
RGT T 1310-73-2 NaOH
PRO Z 948312-77-4
SOL 68-12-2 DMF
NTE Williamson reaction

RX(51) OF 70 COMPOSED OF RX(4), RX(8), RX(14)

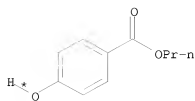
RX(51) F + G + AA ==> AB



F

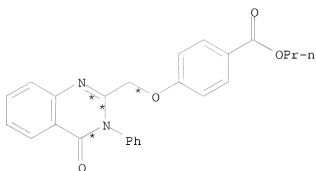


G



AA

3
STEPS
→



AB

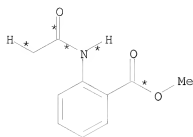
YIELD 29%

RX(4) RCT F 2719-08-6, G 62-53-3
PRO H 2385-23-1
NTE alternative preparation shown

RX(8) RCT H 2385-23-1
RGT N 128-08-5 Bromosuccinimide
PRO M 22312-77-2
CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl3

RX(14) RCT M 22312-77-2, AA 94-13-3
RGT T 1310-73-2 NaOH
PRO AB 948312-78-5
SOL 68-12-2 DMF
NTE Williamson reaction

RX(52) OF 70 COMPOSED OF RX(4), RX(8), RX(15)
RX(52) F + G + AC ==> AD



F

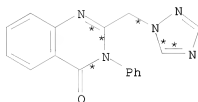


G



AC

3
STEPS
→



AD

YIELD 31%

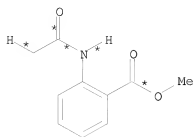
RX(4) RCT F 2719-08-6, G 62-53-3
PRO H 2385-23-1
NTE alternative preparation shown

RX(8) RCT H 2385-23-1
RGT N 128-08-5 Bromosuccinimide
PRO M 22312-77-2
CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl₃

RX(15) RCT M 22312-77-2, AC 288-88-0
PRO AD 948312-72-9
CAT 7440-23-5 Na
SOL 67-56-1 MeOH

RX(53) OF 70 COMPOSED OF RX(4), RX(8), RX(16)

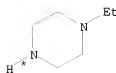
RX(53) F + G + AG ==> AH



F

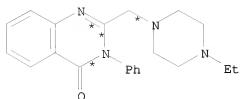


G



AG

3
STEPS
→



AH

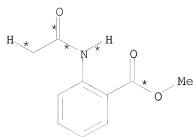
YIELD 24%

RX(4) RCT F 2719-08-6, G 62-53-3
PRO H 2385-23-1
NTE alternative preparation shown

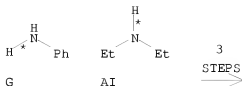
RX(8) RCT H 2385-23-1
RGT N 128-08-5 Bromosuccinimide
PRO M 22312-77-2
CAT 110-86-1 Pyridine
SOL 67-66-3 CHCl3

RX(16) RCT M 22312-77-2, AG 5308-25-8
PRO AH 948312-73-0
CAT 7440-23-5 Na
SOL 67-56-1 MeOH

RX(54) OF 70 COMPOSED OF RX(4), RX(8), RX(17)
RX(54) F + G + AI ==> AJ

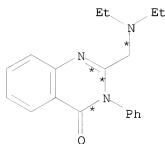


F



G

AI

3
STEPS
→

AJ

YIELD 40%

RX(4) RCT F 2719-08-6, G 62-53-3
 PRO H 2385-23-1
 NTE alternative preparation shown

RX(8) RCT H 2385-23-1
 RGT N 128-08-5 Bromosuccinimide
 PRO M 22312-77-2
 CAT 110-86-1 Pyridine
 SOL 67-66-3 CHCl3

RX(17) RCT M 22312-77-2, AI 109-89-7
 PRO AJ 948312-74-1
 CAT 7440-23-5 Na
 SOL 67-56-1 MeOH

L3 ANSWER 14 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

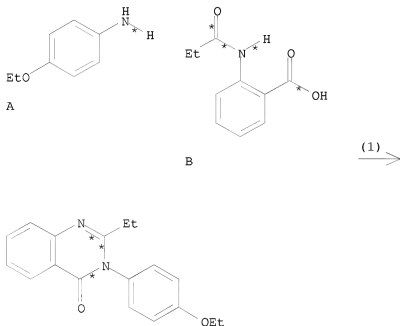
ACCESSION NUMBER: 147:322916 CASREACT

TITLE: Synthesis and structure-activity relationships of
 3H-quinazolin-4-ones and
 3H-pyrido[2,3-d]pyrimidin-4-ones as CXCR3 receptor
 antagonists

AUTHOR(S): Storelli, Stefania; Verzijl, Dennis; Al-Badie, Jawad;

Elders, Niels; Bosch, Leontien; Timmerman, Henk; Smit, Martine J.; De Esch, Iwan J. P.; Leurs, Rob
 CORPORATE SOURCE: Leiden/Amsterdam Center for Drug Research (LACDR),
 Division of Medicinal Chemistry, Faculty of Sciences,
 Vrije Universiteit Amsterdam, Amsterdam, Neth.
 SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2007),
 340(6), 281-291
 CODEN: ARPMAS; ISSN: 0365-6233
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB This study presents the synthesis and initial SAR of CXCR3 antagonists of
 the 3H-quinazolin-4-one and 3H-pyrido[2,3-d]pyrimidin-4-one series. These
 compds. as tools for targeting CXCR3 in a variety of inflammatory models
 are evaluated. Moreover, the structural insights obtained may be used in
 the design of novel CXCR3 antagonists.

RX(1) OF 112 ...A + B ==> C...



C
 YIELD 48%

RX(1) RCT A 156-43-4, B 19165-26-5

STAGE(1)
 RGT D 7719-12-2 PC13
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature -> reflux
 SUBSTAGE(2) 8 hours, reflux
 SUBSTAGE(3) reflux -> room temperature

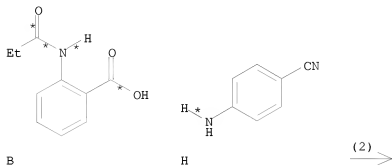
STAGE(2)
 RGT E 497-19-8 Na2CO3

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SOL 7732-18-5 Water
CON room temperature

PRO C 93879-55-1

RX(2) OF 112 ...B + H ==> I...



I
YIELD 35%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

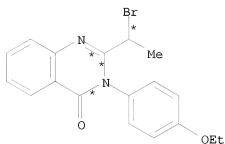
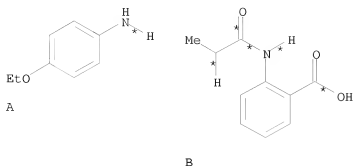
RGT D 7719-12-2 PC13
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> reflux
SUBSTAGE(2) 8 hours, reflux
SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON room temperature

PRO I 860002-79-5

RX(30) OF 112 COMPOSED OF RX(1), RX(4)
RX(30) A + B ==> M



YIELD 96%

RX(1) RCT A 156-43-4, B 19165-26-5

STAGE(1)

RGT D 7719-12-2 PC13
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> reflux
SUBSTAGE(2) 8 hours, reflux
SUBSTAGE(3) reflux -> room temperature

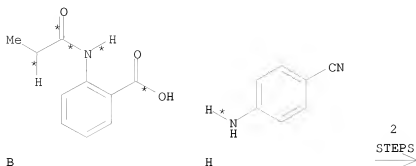
STAGE(2)

RGT E 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON room temperature

PRO C 93879-55-1

RX(4) RCT C 93879-55-1
RGT N 127-09-3 AcONa, O 7726-95-6 Br2
PRO M 876016-38-5
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature -> 40 deg C
SUBSTAGE(2) 3 hours, 40 deg C
NTE regioselective

RX(31) OF 112 COMPOSED OF RX(2), RX(5)
RX(31) B + H ==> Q



Q
YIELD 88%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> reflux
SUBSTAGE(2) 8 hours, reflux
SUBSTAGE(3) reflux -> room temperature

STAGE(2)

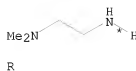
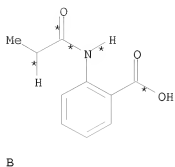
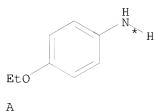
RGT E 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON room temperature

PRO I 860002-79-5

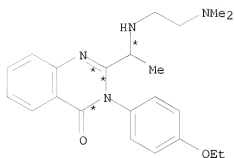
RX(5) RCT I 860002-79-5
RGT N 127-09-3 AcONa, O 7726-95-6 Br2
PRO Q 860002-84-2
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature -> 40 deg C
SUBSTAGE(2) 3 hours, 40 deg C
NTE regioselective

RX(57) OF 112 COMPOSED OF RX(1), RX(4), RX(6)

RX(57) A + B + R ==> S



3
STEPS
→



S
YIELD 52%

RX(1) RCT A 156-43-4, B 19165-26-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

PRO C 93879-55-1

RX(4)

RCT C 93879-55-1

RGT N 127-09-3 AcONa, O 7726-95-6 Br2

PRO M 876016-38-5

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature -> 40 deg C

SUBSTAGE(2) 3 hours, 40 deg C

NTE regioselective

RX(6)

RCT M 876016-38-5, R 108-00-9

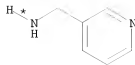
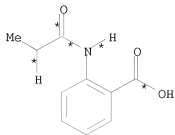
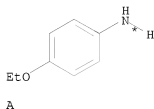
PRO S 947535-98-0

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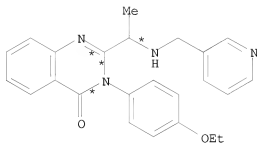
SOL 64-17-5 EtOH
CON 18 hours, reflux

RX(58) OF 112 COMPOSED OF RX(1), RX(4), RX(21)

RX(58) A + B + BE ==> BF



3
STEPS
→



BF
YIELD 40%

RX(1) RCT A 156-43-4, B 19165-26-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

PRO C 93879-55-1

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RX(4) RCT C 93879-55-1
RGT N 127-09-3 AcONa, O 7726-95-6 Br2
PRO M 876016-38-5
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature -> 40 deg C
SUBSTAGE(2) 3 hours, 40 deg C
NTE regioselective

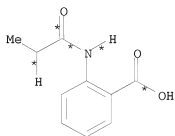
RX(21) RCT BE 3731-52-0

STAGE(1)
RGT X 121-44-8 Et3N
SOL 68-12-2 DMF
CON 0.5 hours, room temperature

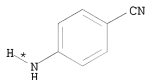
STAGE(2)
RCT M 876016-38-5
CON overnight, room temperature

PRO BF 947536-71-2

RX(61) OF 112 COMPOSED OF RX(2), RX(5), RX(7)
RX(61) B + H + R ==> U



B

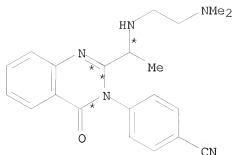


H



R

3
STEPS
→



U
YIELD 47%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> reflux
SUBSTAGE(2) 8 hours, reflux
SUBSTAGE(3) reflux -> room temperature

STAGE(2)

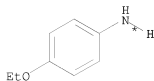
RGT E 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON room temperature

PRO I 860002-79-5

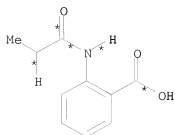
RX(5) RCT I 860002-79-5
RGT N 127-09-3 AcONa, O 7726-95-6 Br2
PRO Q 860002-84-2
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature -> 40 deg C
SUBSTAGE(2) 3 hours, 40 deg C
NTE regioselective

RX(7) RCT Q 860002-84-2, R 108-00-9
PRO U 860002-90-0
SOL 64-17-5 EtOH
CON 18 hours, reflux

RX(67) OF 112 COMPOSED OF RX(1), RX(4), RX(6), RX(13)
RX(67) A + B + R + V ==> AK



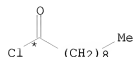
A



B

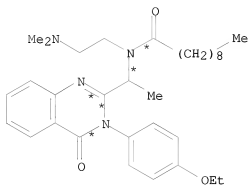


R



V

4
STEPS
→



AK
YIELD 42%

RX(1) RCT A 156-43-4, B 19165-26-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

PRO C 93879-55-1

RX(4) RCT C 93879-55-1
RGT N 127-09-3 AcONa, O 7726-95-6 Br2

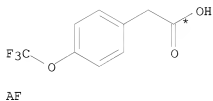
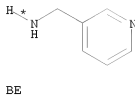
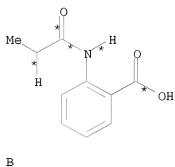
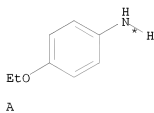
10/ 562,112

PRO M 876016-38-5
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature -> 40 deg C
SUBSTAGE(2) 3 hours, 40 deg C
NTE regioselective

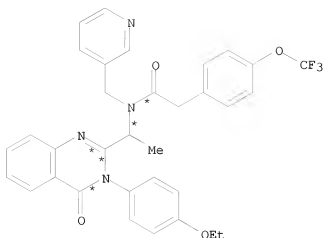
RX(6) RCT M 876016-38-5, R 108-00-9
PRO S 947535-98-0
SOL 64-17-5 EtOH
CON 18 hours, reflux

RX(13) RCT V 112-13-0, S 947535-98-0
RGT X 121-44-8 Et3N
PRO AK 947536-01-8
SOL 123-91-1 Dioxane
CON 18 hours, room temperature

RX(68) OF 112 COMPOSED OF RX(1), RX(4), RX(21), RX(28)
RX(68) A + B + BE + AF ==> BP



4
STEPS
=>



BP

YIELD 59%

RX(1) RCT A 156-43-4, B 19165-26-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

PRO C 93879-55-1

RX(4) RCT C 93879-55-1

RGT N 127-09-3 AcONa, O 7726-95-6 Br2

PRO M 876016-38-5

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature -> 40 deg C

SUBSTAGE(2) 3 hours, 40 deg C

NTE regioselective

RX(21) RCT BE 3731-52-0

STAGE(1)

RGT X 121-44-8 Et3N

SOL 68-12-2 DMF

CON 0.5 hours, room temperature

STAGE(2)

RCT M 876016-38-5

CON overnight, room temperature

PRO BF 947536-71-2

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RX(28) RCT AF 4315-07-5, BF 947536-71-2

STAGE(1)

RGT AH 25952-53-8 EDAP
CAT 68-12-2 DMF
SOL 75-09-2 CH₂Cl₂
CON overnight, room temperature

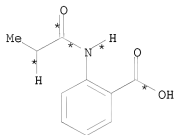
STAGE(2)

RGT AI 144-55-8 NaHCO₃
SOL 7732-18-5 Water
CON room temperature

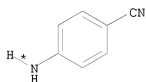
PRO BP 473719-87-8

RX(74) OF 112 COMPOSED OF RX(2), RX(5), RX(7), RX(8)

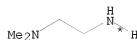
RX(74) B + H + R + V ==> W



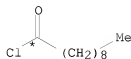
B



H

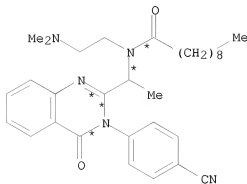


R



V

4
STEPS
→



W
YIELD 35%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13
SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux
 SUBSTAGE(2) 8 hours, reflux
 SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3
 SOL 7732-18-5 Water
 CON room temperature

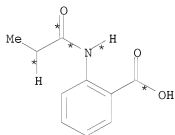
PRO I 860002-79-5

RX(5) RCT I 860002-79-5
 RGT N 127-09-3 AcONa, O 7726-95-6 Br2
 PRO Q 860002-84-2
 SOL 7732-18-5 Water, 64-19-7 AcOH
 CON SUBSTAGE(1) room temperature -> 40 deg C
 SUBSTAGE(2) 3 hours, 40 deg C
 NTE regioselective

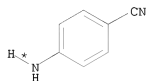
RX(7) RCT Q 860002-84-2, R 108-00-9
 PRO U 860002-90-0
 SOL 64-17-5 EtOH
 CON 18 hours, reflux

RX(8) RCT V 112-13-0, U 860002-90-0
 RGT X 121-44-8 Et3N
 PRO W 860002-95-5
 SOL 123-91-1 Dioxane
 CON 18 hours, room temperature

RX(75) OF 112 COMPOSED OF RX(2), RX(5), RX(7), RX(9)
 RX(75) B + H + R + Z ==> AA



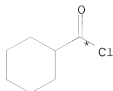
B



H

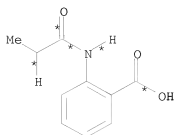


R

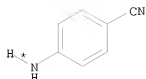


Z

4
 STEPS
 →



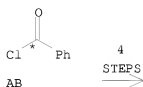
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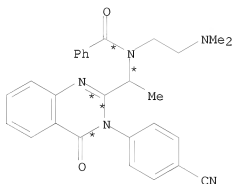
H



R



AB



AC

YIELD 22%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

PRO I 860002-79-5

RX(5) RCT I 860002-79-5

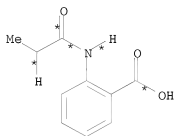
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RGT N 127-09-3 AcONa, O 7726-95-6 Br2
 PRO Q 860002-84-2
 SOL 7732-18-5 Water, 64-19-7 AcOH
 CON SUBSTAGE(1) room temperature -> 40 deg C
 SUBSTAGE(2) 3 hours, 40 deg C
 NTE regioselective

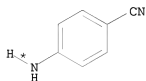
RX(7) RCT Q 860002-84-2, R 108-00-9
 PRO U 860002-90-0
 SOL 64-17-5 EtOH
 CON 18 hours, reflux

RX(10) RCT AB 98-88-4, U 860002-90-0
 RGT X 121-44-8 Et3N
 PRO AC 860003-03-8
 SOL 123-91-1 Dioxane
 CON 18 hours, room temperature

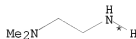
RX(77) OF 112 COMPOSED OF RX(2), RX(5), RX(7), RX(11)
 RX(77) B + H + R + AD ==> AE



B



H

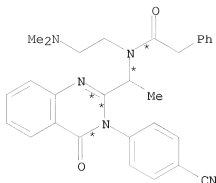


R



AD

4
 STEPS
 →



AE
YIELD 40%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature -> reflux
SUBSTAGE(2) 8 hours, reflux
SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON room temperature

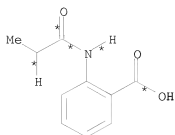
PRO I 860002-79-5

RX(5) RCT I 860002-79-5
RGT N 127-09-3 AcONa, O 7726-95-6 Br2
PRO Q 860002-84-2
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature -> 40 deg C
SUBSTAGE(2) 3 hours, 40 deg C
NTE regioselective

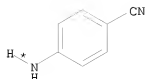
RX(7) RCT Q 860002-84-2, R 108-00-9
PRO U 860002-90-0
SOL 64-17-5 EtOH
CON 18 hours, reflux

RX(11) RCT AD 103-80-0, U 860002-90-0
RGT X 121-44-8 Et3N
PRO AE 947535-99-1
SOL 123-91-1 Dioxane
CON 18 hours, room temperature

RX(78) OF 112 COMPOSED OF RX(2), RX(5), RX(7), RX(12)
RX(78) B + H + R + AF ==> AG



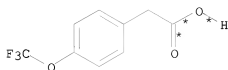
B



H

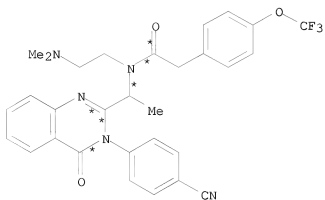


R



AF

4
STEPS
→



AG

YIELD 47%

RX(2) RCT B 19165-26-5, H 873-74-5

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 8 hours, reflux

SUBSTAGE(3) reflux -> room temperature

STAGE(2)

RGT E 497-19-8 Na2CO3

SOL 7732-18-5 Water

CON room temperature

PRO I 860002-79-5

RX(5) RCT I 860002-79-5
RGT N 127-09-3 AcONa, O 7726-95-6 Br2
PRO Q 860002-84-2
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature -> 40 deg C
SUBSTAGE(2) 3 hours, 40 deg C
NTE regioselective

RX(7) RCT Q 860002-84-2, R 108-00-9
PRO U 860002-90-0
SOL 64-17-5 EtOH
CON 18 hours, reflux

RX(12) RCT AF 4315-07-5, U 860002-90-0

STAGE(1)
RGT AH 25952-53-8 EDAP
CAT 68-12-2 DMF
SOL 75-09-2 CH2Cl2
CON overnight, room temperature

STAGE(2)
RGT AI 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON room temperature

PRO AG 947536-00-7

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 147:301069 CASREACT

TITLE: Synthesis and behavior of
2-carboxyvinyl-6,8-dibromo-4H-3,1-benzoxazin-4-one
towards nitrogen, carbon, and sulfur nucleophiles

AUTHOR(S): Abdel-Rahman, T. M.; El-Hashash, M. A.; El-Badry, Y.
A.

CORPORATE SOURCE: Faculty of Specific Education, Ain Shams University,
Cairo, Egypt

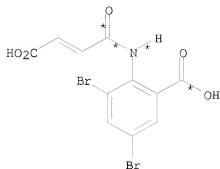
SOURCE: Egyptian Journal of Chemistry (2005), 48(6), 679-693
CODEN: EGJCA3; ISSN: 0449-2285

PUBLISHER: National Information and Documentation Centre

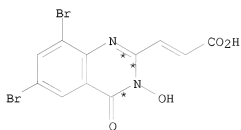
DOCUMENT TYPE: Journal

LANGUAGE: English

AB 3-(6,8-Dibromo-4-oxo-4H-benzo[d][1,3]oxazin-2-yl)acrylic acid (I) was
synthesized and allowed to react with some nitrogen nucleophiles to afford
3-substituted quinazolinones and benzamide derivs.
3-(6,8-Dibromo-3-hydroxy-4-oxo-3,4-dihydroquinazolin-2-yl)acrylic acid was
subjected to acylation and alkylation. Also,
3-(6,8-dibromo-3-(2-hydroxyethyl)-4-oxo-3,4-dihydroquinazolin-2-yl)acrylic
acid was used to alkylate some aromatic systems. Treatment of I with
o-phenylenediamine in different solvents under different conditions
furnished a substituted benzamide and 3-substituted quinazolinone. I was
converted to 4(3H)-quinazolinone by treatment with formamide and/or



C

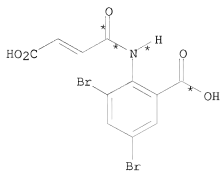
(4) \longrightarrow 

J

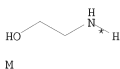
YIELD 73%

RX(4) RCT C 934242-55-4
 RGT K 5470-11-1 H2NOH-HCl
 PRO J 934242-57-6
 SOL 110-86-1 Pyridine
 CON SUBSTAGE(1) 3 hours, reflux
 SUBSTAGE(2) cooled

RX(5) OF 64 ...C + M ==> N...

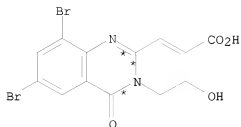


C



M

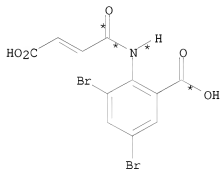
(5) \longrightarrow



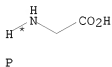
N
YIELD 58%

RX(5) RCT C 934242-55-4, M 141-43-5
 RGT O 127-09-3 AcONa
 PRO N 934242-58-7
 SOL 64-19-7 AcOH
 CON SUBSTAGE(1) 3 hours, reflux
 SUBSTAGE(2) cooled

RX(6) OF 64 ...C + P ==> Q

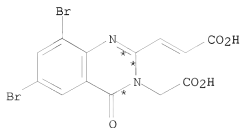


C



P

(6) →

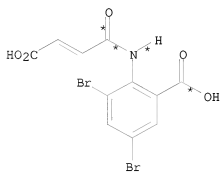


Q
YIELD 44%

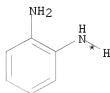
10/ 562,112

RX(6) RCT C 934242-55-4, P 56-40-6
RGT L 110-86-1 Pyridine
PRO Q 934242-59-8
SOL 110-86-1 Pyridine
CON SUBSTAGE(1) 8 hours, reflux
SUBSTAGE(2) cooled

RX(15) OF 64 ...C + AJ ==> AL

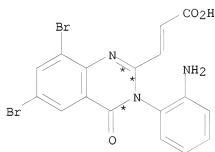


C



AJ

(15) \longrightarrow

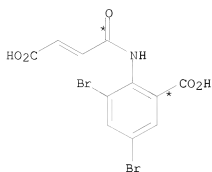


AL
YIELD 56%

RX(15) RCT C 934242-55-4, AJ 95-54-5
RGT O 127-09-3 AcONa
PRO AL 934242-68-9
SOL 64-19-7 AcOH
CON SUBSTAGE(1) 2 hours, reflux
SUBSTAGE(2) cooled
NTE product depends on reaction conditions

RX(16) OF 64 ...C + AM ==> AN...

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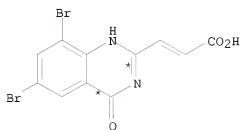


C



AM

(16) \longrightarrow



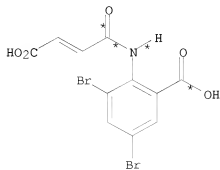
AN

YIELD 65%

RX(16) RCT C 934242-55-4, AM 75-12-7
 PRO AN 934242-69-0
 SOL 75-12-7 Formamide
 CON SUBSTAGE(1) 2 hours, reflux
 SUBSTAGE(2) cooled

RX(44) OF 64 COMPOSED OF RX(4), RX(9)

RX(44) C + F \implies W



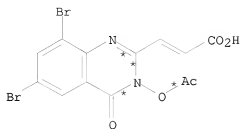
C



F

2
 STEPS
 \longrightarrow

10/ 562,112

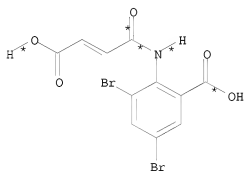


W
YIELD 80%

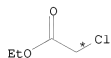
RX(4) RCT C 934242-55-4
RGT K 5470-11-1 H2NOH-HCl
PRO J 934242-57-6
SOL 110-86-1 Pyridine
CON SUBSTAGE(1) 3 hours, reflux
SUBSTAGE(2) cooled

RX(9) RCT J 934242-57-6, F 108-24-7
PRO W 934242-62-3
SOL 108-24-7 Ac2O
CON SUBSTAGE(1) 2 hours, reflux
SUBSTAGE(2) cooled

RX(45) OF 64 COMPOSED OF RX(4), RX(10)
RX(45) C + 2 X ==> Y

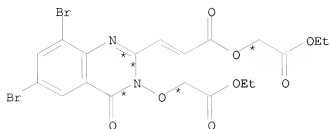


C



2 X

2
STEPS
➔

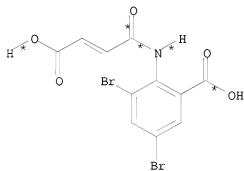


Y
YIELD 28%

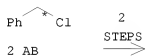
RX(4) RCT C 934242-55-4
RGT K 5470-11-1 H2NOH-HCl
PRO J 934242-57-6
SOL 110-86-1 Pyridine
CON SUBSTAGE(1) 3 hours, reflux
SUBSTAGE(2) cooled

RX(10) RCT J 934242-57-6, X 105-39-5
RGT Z 584-08-7 K2CO3
PRO Y 934242-63-4
SOL 67-64-1 Me2CO
CON 24 hours, reflux

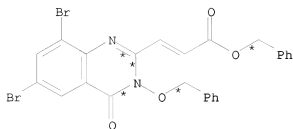
RX(46) OF 64 COMPOSED OF RX(4), RX(11)
RX(46) C + 2 AB ==> AC



C



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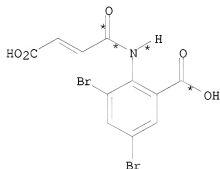


AC
YIELD 37%

RX(4) RCT C 934242-55-4
RGT K 5470-11-1 H2NOH-HCl
PRO J 934242-57-6
SOL 110-86-1 Pyridine
CON SUBSTAGE(1) 3 hours, reflux
SUBSTAGE(2) cooled

RX(11) RCT J 934242-57-6, AB 100-44-7
RGT Z 584-08-7 K2CO3
PRO AC 934242-64-5
SOL 67-64-1 Me2CO
CON 24 hours, reflux

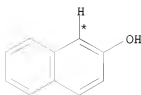
RX(47) OF 64 COMPOSED OF RX(5), RX(12)
RX(47) C + M + AD ==> AE



C

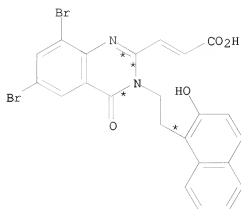


M



AD

2
STEPS
→



AE

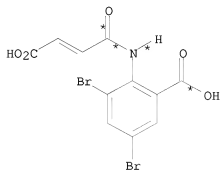
YIELD 38%

RX(5) RCT C 934242-55-4, M 141-43-5
 RGT O 127-09-3 AcONa
 PRO N 934242-58-7
 SOL 64-19-7 AcOH
 CON SUBSTAGE(1) 3 hours, reflux
 SUBSTAGE(2) cooled

 RX(12) RCT N 934242-58-7, AD 135-19-3
 PRO AE 934242-65-6
 CAT 7647-01-0 HCl
 SOL 7732-18-5 Water, 64-17-5 EtOH
 CON SUBSTAGE(1) 6 hours, heated
 SUBSTAGE(2) cooled

RX(48) OF 64 COMPOSED OF RX(5), RX(13)

RX(48) C + M + AH ==> AI



C



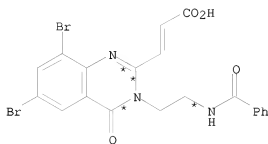
M



AH

10/ 562,112

2
STEPS
→

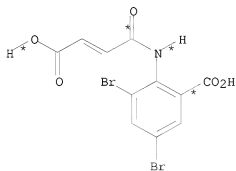


AI
YIELD 44%

RX(5) RCT C 934242-55-4, M 141-43-5
RGT O 127-09-3 AcONa
PRO N 934242-58-7
SOL 64-19-7 AcOH
CON SUBSTAGE(1) 3 hours, reflux
SUBSTAGE(2) cooled

RX(13) RCT N 934242-58-7, AH 55-21-0
PRO AI 934242-66-7
CAT 7647-01-0 HCl
SOL 7732-18-5 Water, 64-17-5 EtOH
CON SUBSTAGE(1) 6 hours, heated
SUBSTAGE(2) cooled

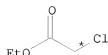
RX(49) OF 64 COMPOSED OF RX(16), RX(17)
RX(49) C + AM + 2 X ==> AO



C



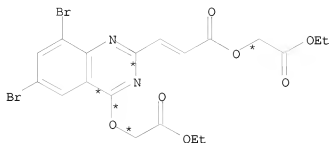
AM



2 X

10/ 562,112

2
STEPS
→

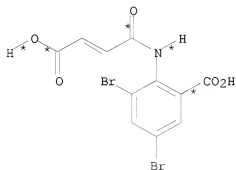


AO
YIELD 32%

RX(16) RCT C 934242-55-4, AM 75-12-7
PRO AN 934242-69-0
SOL 75-12-7 Formamide
CON SUBSTAGE(1) 2 hours, reflux
SUBSTAGE(2) cooled

RX(17) RCT X 105-39-5, AN 934242-69-0
RGT Z 584-08-7 K2CO3
PRO AO 934242-70-3
SOL 67-64-1 Me2CO
CON 25 hours, reflux

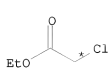
RX(63) OF 64 COMPOSED OF RX(16), RX(17), RX(18)
RX(63) C + AM + 2 X ==> AP



C

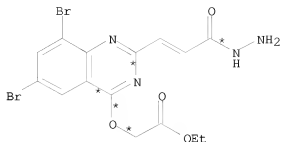


AM



2 X

3
STEPS
→



AP
YIELD 57%

RX(16) RCT C 934242-55-4, AM 75-12-7
PRO AN 934242-69-0
SOL 75-12-7 Formamide
CON SUBSTAGE(1) 2 hours, reflux
SUBSTAGE(2) cooled

RX(17) RCT X 105-39-5, AN 934242-69-0
RGT Z 584-08-7 K2CO3
PRO AO 934242-70-3
SOL 67-64-1 Me2CO
CON 25 hours, reflux

RX(18) RCT AO 934242-70-3
RGT AQ 7803-57-8 N2H4-H2O
PRO AP 934242-71-4
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 6 hours, reflux
SUBSTAGE(2) cooled

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 16 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 147:277558 CASREACT

TITLE: Synthesis, characterization, chelating properties and anti-fungal activity of 2-(4-phenylpiperazinyl)methyl-3-(8-quinolinol-5-yl)-4(3H)-quinazolinone

AUTHOR(S): Shelat, C. D.; Vashi, R. T.

CORPORATE SOURCE: Department of Chemistry, Navyug Science College, Surat, 395 000, India

SOURCE: E-Journal of Chemistry (2005), 2(6), 86-90

CODEN: ECJHAO

URL: <http://cc.lasphost.com/namfarook/NEWEJC/VOL2/SIXTH/fulltext/86-90.pdf>

PUBLISHER: WWW Publications

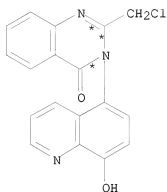
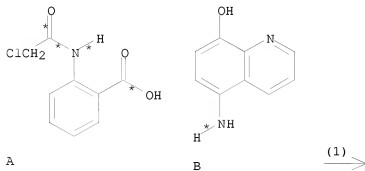
DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

AB Title compds. were prepared from 2-HO2CC6H4NHC(=O)CH2Cl, 5-amino-8-quinolinol,

and N-phenylpiperazine and characterized. Various transition metal (Cu^{2+} , Co^{2+} , Ni^{2+} , Zn^{2+} , Mn^{2+}) chelates were prepared and characterized by metal ligand (M:L) ratio, IR and reflectance spectral studies, magnetic moment, and antimicrobial activity.

RX(1) OF 18 A + B ==> C...



RX(1) RCT A 14422-49-2, B 13207-66-4

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 9 hours, reflux

STAGE(2)

RGT E 7732-18-5 Water

CON cooled

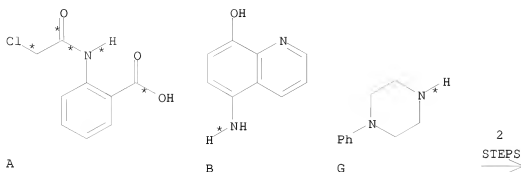
PRO C 946052-78-4

NTE regioselective

RX(8) OF 18 COMPOSED OF RX(1), RX(2)

RX(8) A + B + G ==> H

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H
YIELD 80%

RX(1) RCT A 14422-49-2, B 13207-66-4

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 9 hours, reflux

STAGE(2)

RGT E 7732-18-5 Water

CON cooled

PRO C 946052-78-4

NTE regioselective

RX(2) RCT C 946052-78-4, G 92-54-6

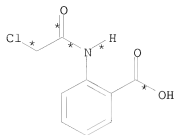
PRO H 946052-79-5

SOL 110-86-1 Pyridine

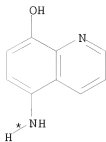
CON 10 hours, reflux

RX(14) OF 18 COMPOSED OF RX(1), RX(2), RX(3)

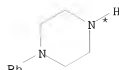
RX(14) 2 A + 2 B + 2 G ==> J



2 A



2 B

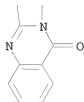


2 G

3
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



J
YIELD 83%

RX(1) RCT A 14422-49-2, B 13207-66-4

STAGE(1)

RGT D 7719-12-2 PC13
SOL 108-88-3 PhMe
CON 9 hours, reflux

STAGE(2)

RGT E 7732-18-5 Water
CON cooled

PRO C 946052-78-4
NTE regioselective

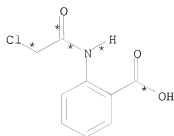
RX(2) RCT C 946052-78-4, G 92-54-6
PRO H 946052-79-5
SOL 110-86-1 Pyridine
CON 10 hours, reflux

RX(3) RCT H 946052-79-5
RGT K 127-09-3 AcONa, L 64-18-6 HCO2H, M 142-71-2 Cu(OAc)2
PRO J 946052-80-8
SOL 7732-18-5 Water
CON 2 hours, heated

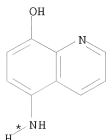
RX(15) OF 18 COMPOSED OF RX(1), RX(2), RX(4)

10/ 562,112

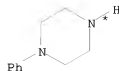
RX(15) 2 A + 2 B + 2 G ==> N



2 A



2 B

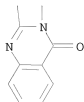


2 G

3
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



N
YIELD 89%

RX(1) RCT A 14422-49-2, B 13207-66-4

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 9 hours, reflux

STAGE(2)

RGT E 7732-18-5 Water

CON cooled

PRO C 946052-78-4

NTE regioselective

RX(2) RCT C 946052-78-4, G 92-54-6

PRO H 946052-79-5

SOL 110-86-1 Pyridine

CON 10 hours, reflux

RX(4) RCT H 946052-79-5

RGT O 71-48-7 Co(OAc)2, K 127-09-3 AcONa, L 64-18-6 HCO2H

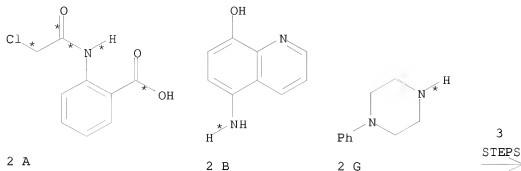
PRO N 946052-81-9

SOL 7732-18-5 Water

CON 2 hours, heated

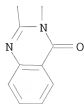
10/ 562,112

RX(16) OF 18 COMPOSED OF RX(1), RX(2), RX(5)
RX(16) 2 A + 2 B + 2 G ==> P



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



P
YIELD 79%

RX(1) RCT A 14422-49-2, B 13207-66-4

STAGE(1)

RGT D 7719-12-2 PC13
SOL 108-88-3 PhMe
CON 9 hours, reflux

STAGE(2)

RGT E 7732-18-5 Water
CON cooled

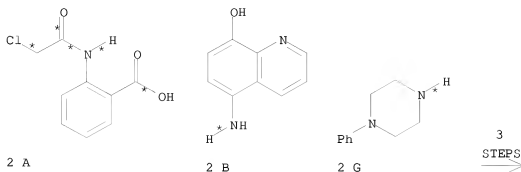
PRO C 946052-78-4
NTE regioselective

RX(2) RCT C 946052-78-4, G 92-54-6
PRO H 946052-79-5
SOL 110-86-1 Pyridine
CON 10 hours, reflux

RX(5) RCT H 946052-79-5
RGT Q 373-02-4 Ni(OAc)₂, K 127-09-3 AcONa, L 64-18-6 HCO₂H
PRO P 946052-82-0
SOL 7732-18-5 Water
CON 2 hours, heated

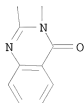
10/ 562,112

RX(17) OF 18 COMPOSED OF RX(1), RX(2), RX(6)
RX(17) 2 A + 2 B + 2 G ==> R



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



R
YIELD 86%

RX(1) RCT A 14422-49-2, B 13207-66-4

STAGE(1)

RGT D 7719-12-2 PC13
SOL 108-88-3 PhMe
CON 9 hours, reflux

STAGE(2)

RGT E 7732-18-5 Water
CON cooled

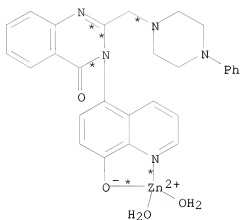
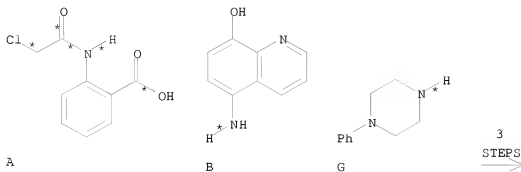
PRO C 946052-78-4
NTE regioselective

RX(2) RCT C 946052-78-4, G 92-54-6
PRO H 946052-79-5
SOL 110-86-1 Pyridine
CON 10 hours, reflux

RX(6) RCT H 946052-79-5
RGT S 638-38-0 Mn(OAc)2, K 127-09-3 AcONa, L 64-18-6 HCO2H
PRO R 946052-83-1
SOL 7732-18-5 Water
CON 2 hours, heated

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RX(18) OF 18 COMPOSED OF RX(1), RX(2), RX(7)
 RX(18) A + B + G ==> T



T
 YIELD 88%

RX(1) RCT A 14422-49-2, B 13207-66-4

STAGE(1)

RGT D 7719-12-2 PC13
 SOL 108-88-3 PhMe
 CON 9 hours, reflux

STAGE(2)

RGT E 7732-18-5 Water
 CON cooled

PRO C 946052-78-4
 NTE regioselective

RX(2) RCT C 946052-78-4, G 92-54-6
 PRO H 946052-79-5
 SOL 110-86-1 Pyridine
 CON 10 hours, reflux

RX(7) RCT H 946052-79-5
RGT U 557-34-6 Zn(OAc)2, K 127-09-3 AcONa, L 64-18-6 HCO2H
PRO T 946052-84-2
SOL 7732-18-5 Water
CON 2 hours, heated

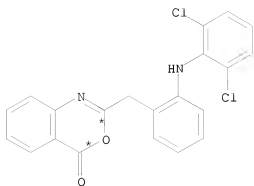
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 17 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 147:235107 CASREACT
TITLE: Quinazolin-4(3H)-ones of
2-[(2',6'-dichlorophenyl)amino]phenyl acetic acid with
substituted aryl acetamide and their microbial studies
AUTHOR(S): Patel, N. B.; Chaudhari, R. C.
CORPORATE SOURCE: Department of Chemistry, Veer Narmad South Gujarat
University, Surat, 395 007, India
SOURCE: Journal of the Indian Chemical Society (2006), 83(8),
838-841
CODEN: JICSAH; ISSN: 0019-4522
PUBLISHER: Indian Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

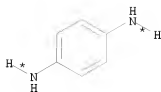
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Synthesis and antimicrobial activity of quinazolinones I (X = 1,4-C6H4,
bond; R = H, 2-NO2, 3-NO2, 4-NO2, 2-Me, 3-Me, 4-Me, 2-MeO, 4-MeO, 2-Cl,
3-Cl, 4-Cl; R1 = H, Br) were reported from
[(2,6-dichlorophenyl)amino]phenylacetic acid and appropriate
N-arylacetamides via benzoxazine II (R = H, Br). All the compds. were
established on the basis of spectral data (IR, 1H NMR) and elemental anal.

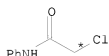
RX(1) OF 48 A + B + C ==> D



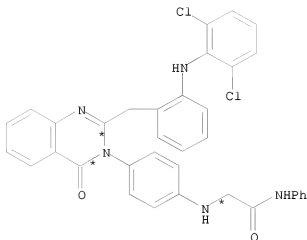
A



B



C



D
YIELD 31%

RX(1) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

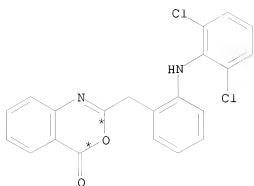
RCT C 587-65-5

SOL 67-56-1 MeOH

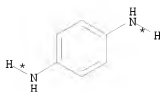
CON reflux

PRO D 945486-73-7

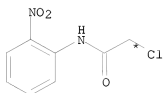
RX(2) OF 48 A + B + G ==> H



A



B



G



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

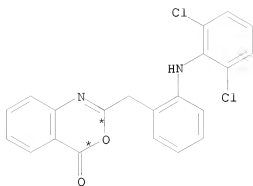
RCT G 10147-70-3

SOL 67-56-1 MeOH

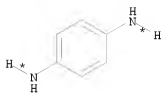
CON reflux

PRO H 945486-74-8

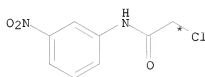
RX(3) OF 48 A + B + I ==> J



A



B



I



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(3) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

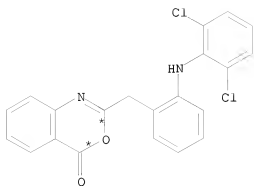
RCT I 10147-71-4

SOL 67-56-1 MeOH

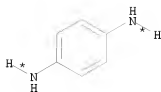
CON reflux

PRO J 945486-75-9

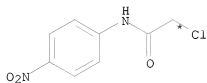
RX(4) OF 48 A + B + K ==> L



A



B



K



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(4) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

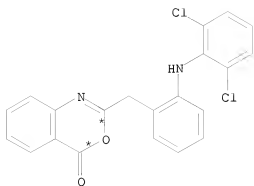
RCT K 17329-87-2

SOL 67-56-1 MeOH

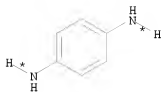
CON reflux

PRO L 945486-76-0

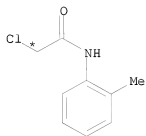
RX(5) OF 48 A + B + M ==> N



A



B



M



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(5) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

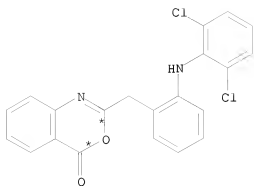
RCT M 37394-93-7

SOL 67-56-1 MeOH

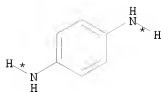
CON reflux

PRO N 945486-77-1

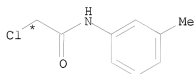
RX(6) OF 48 A + B + O ==> P



A



B



O



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(6) RCT A 402950-18-9, B 106-50-3

STAGE(1)

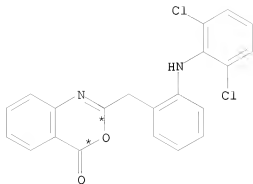
SOL 110-86-1 Pyridine
CON reflux

STAGE(2)

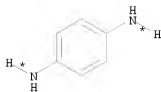
RCT O 32428-61-8
SOL 67-56-1 MeOH
CON reflux

PRO P 945486-78-2

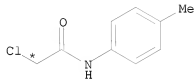
RX(7) OF 48 A + B + Q ==> R



A



B



Q



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(7) RCT A 402950-18-9, B 106-50-3

STAGE(1)

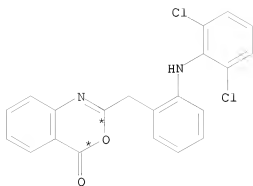
SOL 110-86-1 Pyridine
CON reflux

STAGE(2)

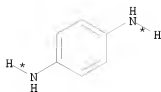
RCT Q 16634-82-5
SOL 67-56-1 MeOH
CON reflux

PRO R 945486-79-3

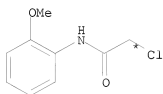
RX(8) OF 48 A + B + S ==> T



A



B



S



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(8) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

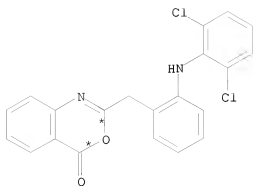
RCT S 55860-22-5

SOL 67-56-1 MeOH

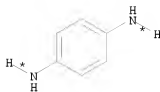
CON reflux

PRO T 945486-80-6

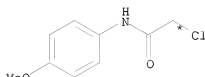
RX(9) OF 48 A + B + U ==> V



A



B



U

(9)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(9) RCT A 402950-18-9, B 106-50-3

STAGE(1)

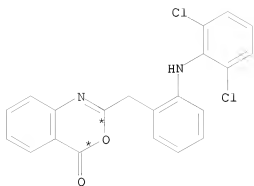
SOL 110-86-1 Pyridine
CON reflux

STAGE(2)

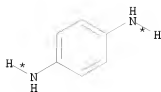
RCT U 22303-36-2
SOL 67-56-1 MeOH
CON reflux

PRO V 945486-81-7

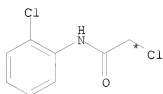
RX(10) OF 48 A + B + W ==> X



A



B



W

(10) \longrightarrow

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(10) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT W 3289-76-7

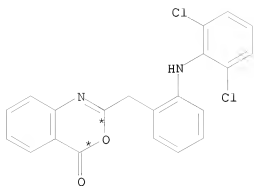
SOL 67-56-1 MeOH

CON reflux

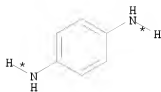
PRO X 945486-82-8

RX(11) OF 48 A + B + Y ==> Z

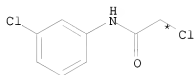
10/ 562,112



A



B



Y



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

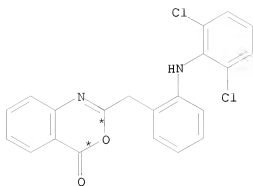
RX(11) RCT A 402950-18-9, B 106-50-3

STAGE(1)
SOL 110-86-1 Pyridine
CON reflux

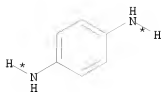
STAGE(2)
RCT Y 2564-05-8
SOL 67-56-1 MeOH
CON reflux

PRO Z 945486-83-9

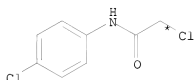
RX(12) OF 48 A + B + AA ==> AB



A



B



AA

(12) →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(12) RCT A 402950-18-9, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

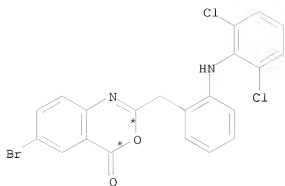
RCT AA 3289-75-6

SOL 67-56-1 MeOH

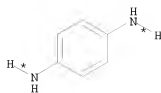
CON reflux

PRO AB 945486-84-0

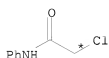
RX(13) OF 48 AC + B + C ==> AD



AC

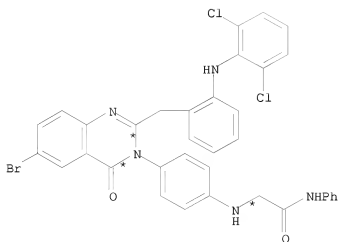


B



C

(13)



AD

YIELD 39%

RX(13) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine
CON reflux

STAGE(2)

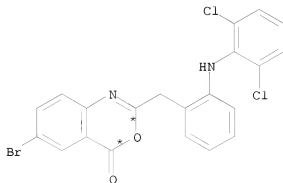
RCT C 587-65-5
SOL 67-56-1 MeOH

10/ 562,112

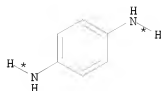
CON reflux

PRO AD 945486-85-1

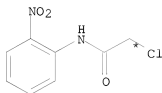
RX(14) OF 48 AC + B + G ==> AE



AC



B



G

(14)
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(14) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

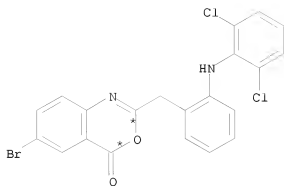
RCT G 10147-70-3

SOL 67-56-1 MeOH

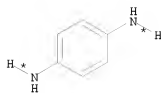
CON reflux

PRO AE 945486-86-2

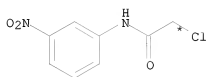
RX(15) OF 48 AC + B + I ==> AF



AC



B



I

(15)
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(15) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

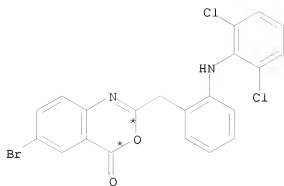
RCT I 10147-71-4

SOL 67-56-1 MeOH

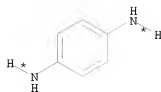
CON reflux

PRO AF 945486-87-3

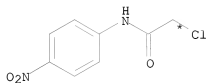
RX(16) OF 48 AC + B + K ==> AG



AC



B



K

(16) →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(16) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

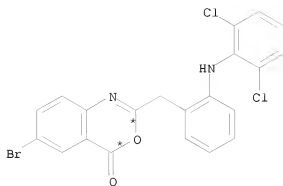
RCT K 17329-87-2

SOL 67-56-1 MeOH

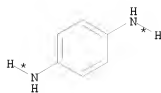
CON reflux

PRO AG 945486-88-4

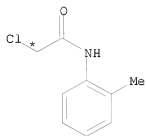
RX(17) OF 48 AC + B + M ==> AH



AC



B



M



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(17) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

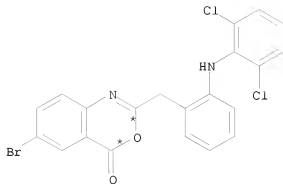
RCT M 37394-93-7

SOL 67-56-1 MeOH

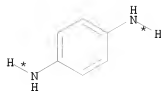
CON reflux

PRO AH 945486-89-5

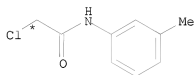
RX(18) OF 48 AC + B + O ==> AI



AC



B



O

(18)
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(18) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

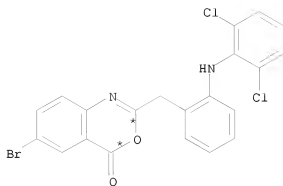
SOL 110-86-1 Pyridine
CON reflux

STAGE(2)

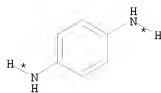
RCT O 32428-61-8
SOL 67-56-1 MeOH
CON reflux

PRO AI 945486-90-8

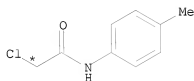
RX(19) OF 48 AC + B + Q ==> AJ



AC



B



Q

(19)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(19) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

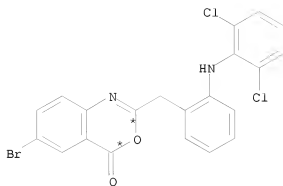
SOL 110-86-1 Pyridine
CON reflux

STAGE(2)

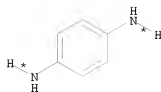
RCT Q 16634-82-5
SOL 67-56-1 MeOH
CON reflux

PRO AJ 945486-91-9

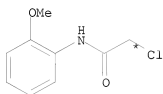
RX(20) OF 48 AC + B + S ==> AK



AC



B



S

(20)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(20) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

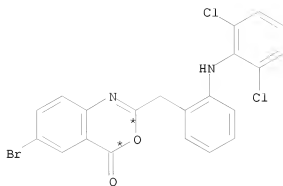
RCT S 55860-22-5

SOL 67-56-1 MeOH

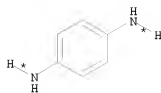
CON reflux

PRO AK 945486-92-0

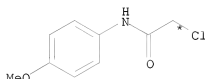
RX(21) OF 48 AC + B + U ==> AL



AC



B



U

(21)
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(21) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

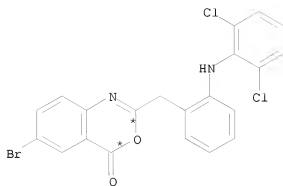
SOL 110-86-1 Pyridine
CON reflux

STAGE(2)

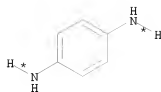
RCT U 22303-36-2
SOL 67-56-1 MeOH
CON reflux

PRO AL 945486-93-1

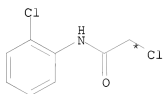
RX(22) OF 48 AC + B + W ==> AM



AC



B



W

(22)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(22) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

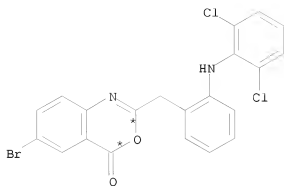
RCT W 3289-76-7

SOL 67-56-1 MeOH

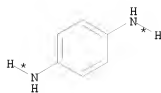
CON reflux

PRO AM 945486-94-2

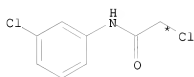
RX(23) OF 48 AC + B + Y ==> AN



AC



B



Y

(23)
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(23) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

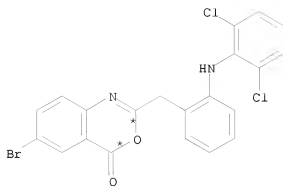
RCT Y 2564-05-8

SOL 67-56-1 MeOH

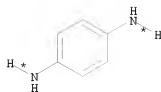
CON reflux

PRO AN 945486-95-3

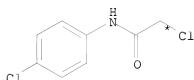
RX(24) OF 48 AC + B + AA ==> AO



AC



B



AA

(24) →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(24) RCT AC 945487-25-2, B 106-50-3

STAGE(1)

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT AA 3289-75-6

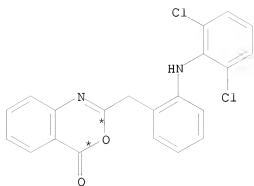
SOL 67-56-1 MeOH

CON reflux

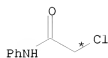
PRO AO 945486-96-4

RX(25) OF 48 A + C ==> AP

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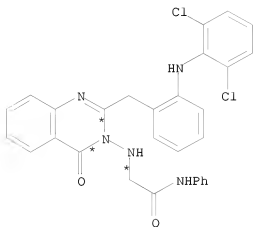


A



C

(25)



AP

YIELD 40%

RX(25) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

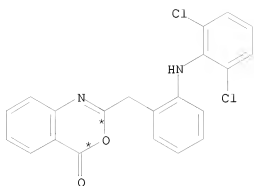
RCT C 587-65-5

SOL 67-56-1 MeOH

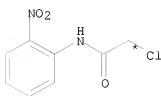
CON reflux

PRO AP 945486-97-5

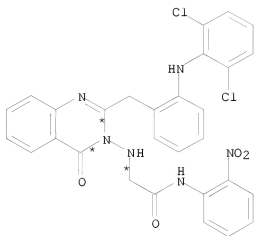
RX(26) OF 48 A + G ==> AR



A



G

(26) \longrightarrow AR
YIELD 46%

RX(26) RCT A 402950-18-9

STAGE(1)

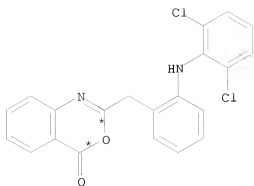
RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine
CON reflux

STAGE(2)

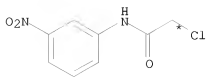
RCT G 10147-70-3
SOL 67-56-1 MeOH
CON reflux

PRO AR 945486-98-6

RX(27) OF 48 A + I ==> AS

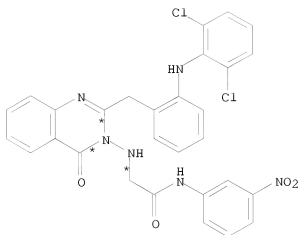


A



I

(27) →



AS
YIELD 44%

RX(27) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine
CON reflux

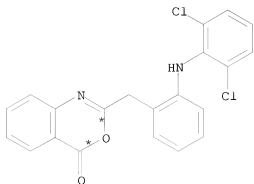
STAGE(2)

RCT I 10147-71-4
SOL 67-56-1 MeOH
CON reflux

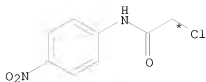
PRO AS 945486-99-7

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RX(28) OF 48 A + K ==> AT

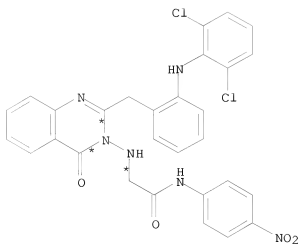


A



K

(28)
→



AT

YIELD 44%

RX(28) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine
CON reflux

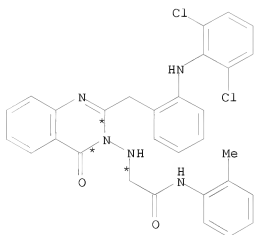
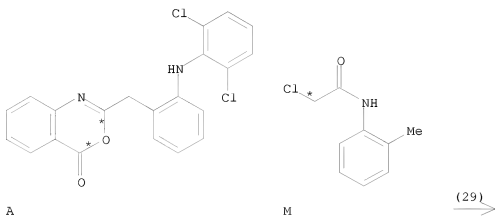
STAGE(2)

RCT K 17329-87-2
SOL 67-56-1 MeOH
CON reflux

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PRO AT 945487-00-3

RX(29) OF 48 A + M ==> AU



AU
YIELD 56%

RX(29) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine
CON reflux

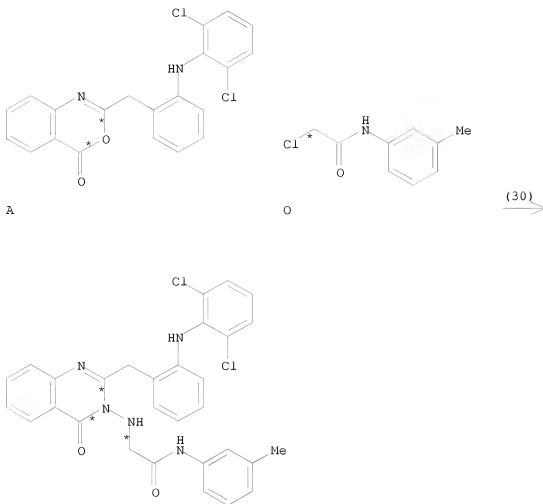
STAGE(2)

RCT M 37394-93-7
SOL 67-56-1 MeOH
CON reflux

PRO AU 945487-01-4

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RX(30) OF 48 A + O ==> AV



AV
YIELD 51%

RX(30) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT O 32428-61-8

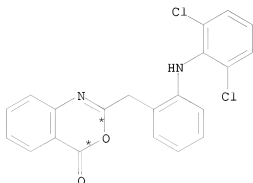
SOL 67-56-1 MeOH

CON reflux

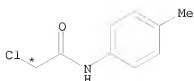
PRO AV 945487-02-5

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RX(31) OF 48 A + Q ==> AW

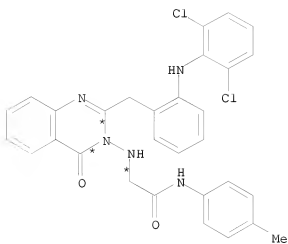


A



Q

(31) 



AW

YIELD 39%

RX(31) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

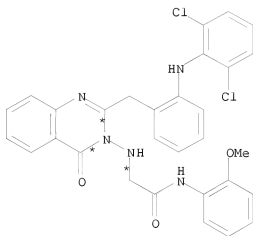
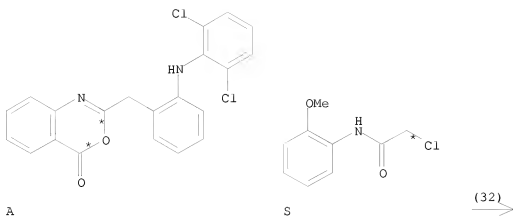
RCT Q 16634-82-5

SOL 67-56-1 MeOH

CON reflux

PRO AW 945487-03-6

RX(32) OF 48 A + S ==> AX



AX
YIELD 62%

RX(32) RCT A 402950-18-9

STAGE(1)

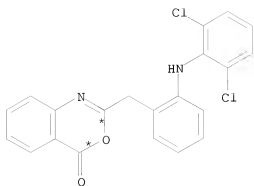
RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine
CON reflux

STAGE(2)

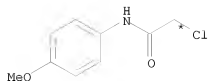
RCT S 55860-22-5
SOL 67-56-1 MeOH
CON reflux

PRO AX 945487-04-7

RX(33) OF 48 A + U ==> AY

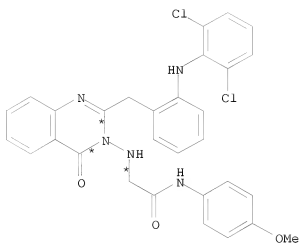


A



U

(33) 



AY

YIELD 63%

RX(33) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine
CON reflux

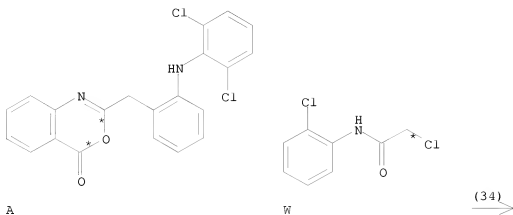
STAGE(2)

RCT U 22303-36-2
SOL 67-56-1 MeOH
CON reflux

PRO AY 945487-05-8

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RX(34) OF 48 A + W ==> AZ



AZ
YIELD 46%

RX(34) RCT A 402950-18-9

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

RCT W 3289-76-7

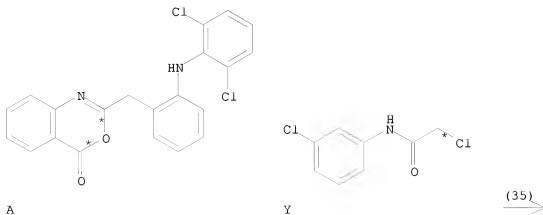
SOL 67-56-1 MeOH

CON reflux

PRO AZ 945487-06-9

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RX(35) OF 48 A + Y ==> BA



BA
YIELD 45%

RX(35) RCT A 402950-18-9

STAGE(1)

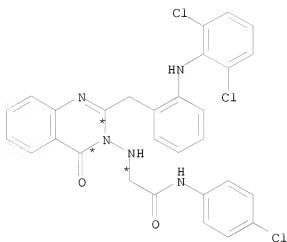
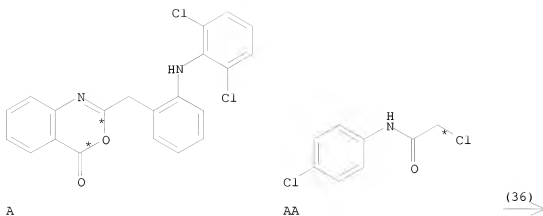
RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine
CON reflux

STAGE(2)

RCT Y 2564-05-8
SOL 67-56-1 MeOH
CON reflux

PRO BA 945487-07-0

RX(36) OF 48 A + AA ==> BB



BB
YIELD 45%

RX(36) RCT A 402950-18-9

STAGE(1)

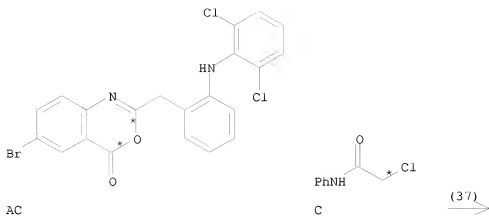
RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine
CON reflux

STAGE(2)

RCT AA 3289-75-6
SOL 67-56-1 MeOH
CON reflux

PRO BB 945487-08-1

RX(37) OF 48 AC + C ==> BC



BC
YIELD 42%

RX(37) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine
CON reflux

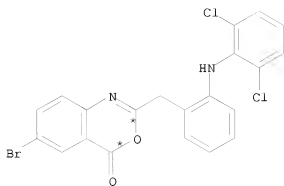
STAGE(2)

RCT C 587-65-5
SOL 67-56-1 MeOH
CON reflux

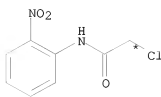
PRO BC 945487-09-2

RX(38) OF 48 AC + G ==> BD

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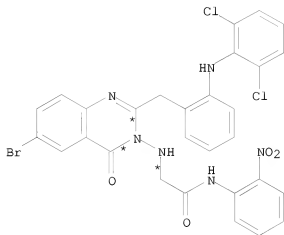


AC



G

(38) \longrightarrow



BD

YIELD 47%

RX(38) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

CON reflux

STAGE(2)

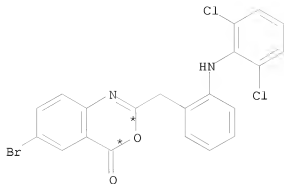
RCT G 10147-70-3

SOL 67-56-1 MeOH

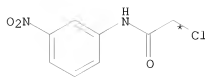
CON reflux

PRO BD 945487-10-5

RX(39) OF 48 AC + I ==> BE

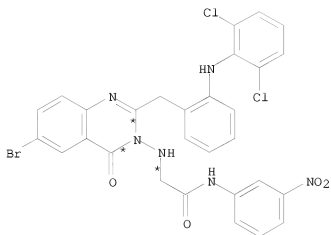


AC



I

(39) →



BE

YIELD 49%

RX(39) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine
CON reflux

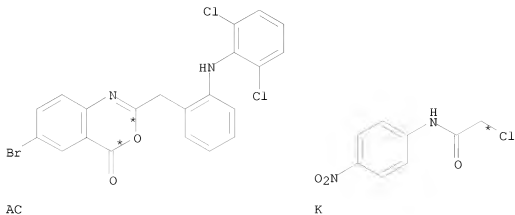
STAGE(2)

RCT I 10147-71-4
SOL 67-56-1 MeOH
CON reflux

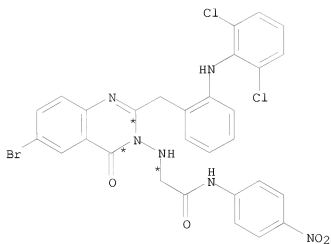
PRO BE 945487-11-6

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RX(40) OF 48 AC + K ==> BF



(40)



BF
YIELD 41%

RX(40) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine
CON reflux

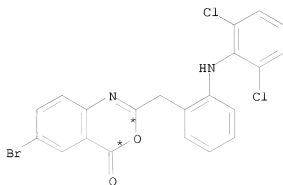
STAGE(2)

RCT K 17329-87-2
SOL 67-56-1 MeOH
CON reflux

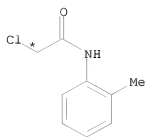
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PRO BF 945487-12-7

RX(41) OF 48 AC + M ==> BG

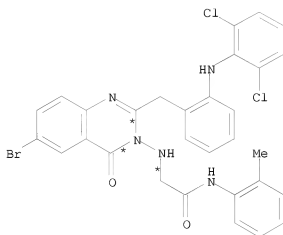


AC



M

(41) →



BG

YIELD 33%

RX(41) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine
CON reflux

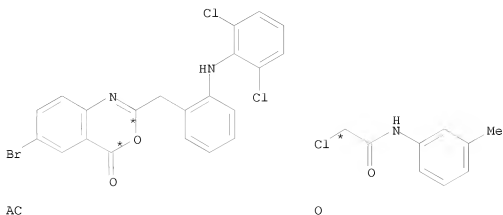
STAGE(2)

RCT M 37394-93-7
SOL 67-56-1 MeOH
CON reflux

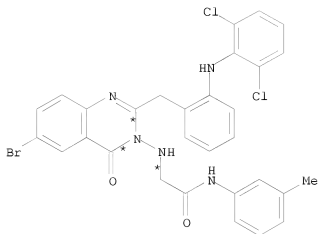
PRO BG 945487-13-8

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RX(42) OF 48 AC + O ==> BH



(42)



BH
YIELD 39%

RX(42) RCT AC 945487-25-2

STAGE(1)

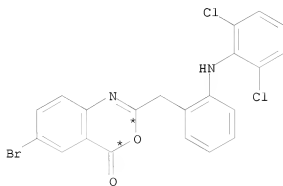
RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine
CON reflux

STAGE(2)

RCT O 32428-61-8
SOL 67-56-1 MeOH
CON reflux

PRO BH 945487-14-9

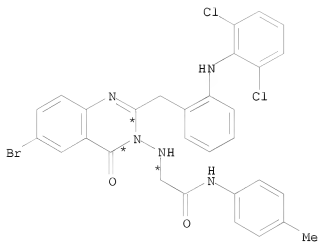
RX(43) OF 48 AC + Q ==> BI



AC

Q

(43) →



BI

YIELD 38%

RX(43) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

STAGE(2)

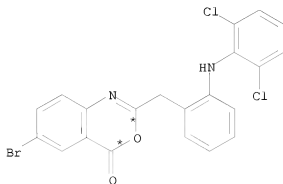
RCT Q 16634-82-5

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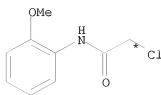
SOL 67-56-1 MeOH

PRO BI 945487-15-0

RX(44) OF 48 AC + S ==> BJ

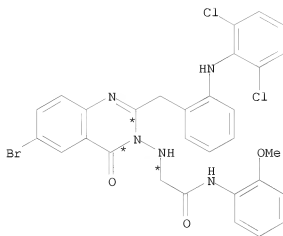


AC



S

(44)
→



BJ

YIELD 63%

RX(44) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

STAGE(2)

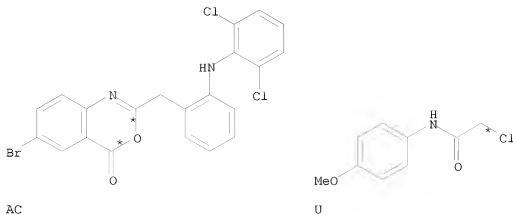
RCT S 55860-22-5

SOL 67-56-1 MeOH

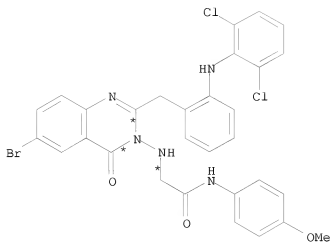
PRO BJ 945487-16-1

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RX(45) OF 48 AC + U ==> BK



(45)



BK
YIELD 66%

RX(45) RCT AC 945487-25-2

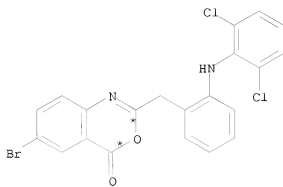
STAGE(1)
RGT AQ 7803-57-8 N2H4-H2O
SOL 110-86-1 Pyridine

STAGE(2)
RCT U 22303-36-2
SOL 67-56-1 MeOH

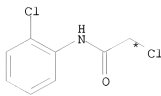
PRO BK 945487-17-2

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RX(46) OF 48 AC + W ==> BL

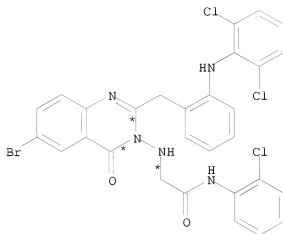


AC



W

(46)



BL

YIELD 36%

RX(46) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

STAGE(2)

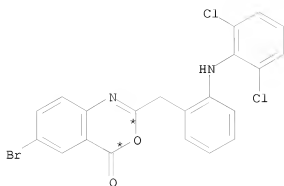
RCT W 3289-76-7

SOL 67-56-1 MeOH

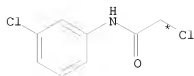
PRO BL 945487-18-3

RX(47) OF 48 AC + Y ==> BM

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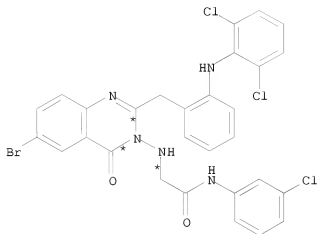


AC



Y

(47)



BM

YIELD 37%

RX(47) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

STAGE(2)

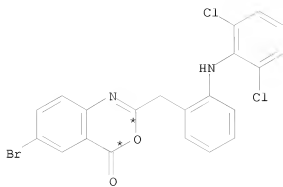
RCT Y 2564-05-8

SOL 67-56-1 MeOH

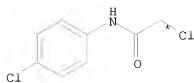
PRO BM 945487-19-4

RX(48) OF 48 AC + AA ==> BN

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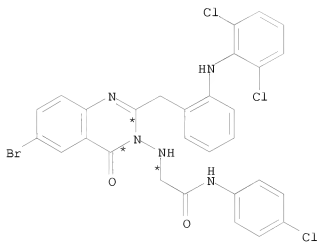


AC



AA

(48)
→



BN

YIELD 40%

RX(48) RCT AC 945487-25-2

STAGE(1)

RGT AQ 7803-57-8 N2H4-H2O

SOL 110-86-1 Pyridine

STAGE(2)

RCT AA 3289-75-6

SOL 67-56-1 MeOH

PRO BN 945487-22-9

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 18 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 147:211826 CASREACT

TITLE: Discovery and optimization of a series of quinazolinone-derived antagonists of CXCR3
 AUTHOR(S): Johnson, Michael; Li, An-Rong; Liu, Jiwen; Fu, Zice; Zhu, Liusheng; Miao, Shichang; Wang, Xuemei; Xu, Qingge; Huang, Alan; Marcus, Andrew; Xu, Feng; Ebsworth, Karen; Sablan, Emmanuel; Danao, Jay; Kumer, Jeff; Dairaghi, Dan; Lawrence, Chris; Sullivan, Tim; Tonn, George; Schall, Thomas; Collins, Tassie; Medina, Julio

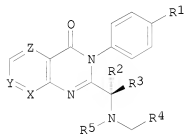
CORPORATE SOURCE: Amgen Inc., South San Francisco, CA, 94080, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(12), 3339-3343
 CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

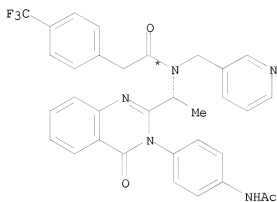
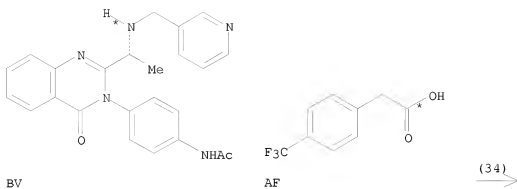
GI



I

AB A series of quinazolinone-derived inhibitors of the CXCR3 receptor I (X, Y, Z = CH, N; R1 = H, F, Cl, EtO, MeC.tplbond.C, etc.; R2 = R3 = H, Me; R2 = H, R3 = Me, Et, Ph; R4 = Me2NCH2, EtOCH2, 3-pyridyl, etc.; R5 = n-octyl, 4-F3CC6H4CH2CO, n-C8H17SO2, etc.) have been synthesized and their affinity for the receptor evaluated. These compds. were evaluated in a 125I-IP10 displacement assay and in in vitro cell migration assays to IP10, ITAC, and MIG using human peripheral blood mononuclear cells.

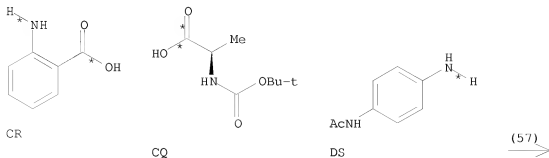
RX(34) OF 342 ...BV + AF ==> BW



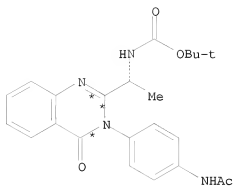
BW
YIELD 90%

RX(34) RCT BV 944915-81-5, AF 32857-62-8
RGT D 2592-95-2 1-Benzotriazolol, E 25952-53-8 EDAP
PRO BW 944915-21-3
SOL 68-12-2 DMF
CON 1 hour, room temperature

RX(57) OF 342 CR + CQ + DS ==> DT...



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DT
YIELD 50%

RX(57) RCT CR 118-92-3, CQ 7764-95-6

STAGE(1)

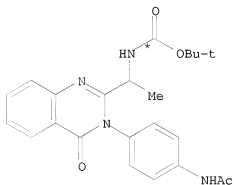
RGT U 110-86-1 Pyridine, CZ 101-02-0 P(OPh)₃
CON 3 hours, 70 deg C

STAGE(2)

RCT DS 122-80-5
CON 1 hour, 55 deg C

PRO DT 944915-41-7

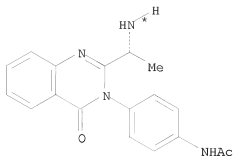
RX(73) OF 342 ...DT ==> EO...



DT

(73)
→

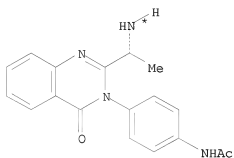
10/ 562,112



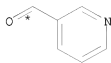
EO
YIELD 90%

RX(73) RCT DT 944915-41-7
 RGT ED 76-05-1 F3CCO2H
 PRO EO 944915-56-4
 SOL 75-09-2 CH2Cl2
 CON 2 hours, room temperature

RX(98) OF 342 ...EO + FC ==> BV...

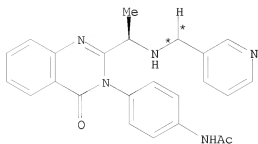


EO



FC

(98) \rightarrow

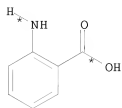


BV
YIELD 80%

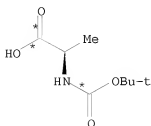
10/ 562,112

RX(98) RCT EO 944915-56-4, FC 500-22-1
RGT O 56553-60-7 Na.(AcO)3BH
PRO BV 944915-81-5
SOL 107-06-2 ClCH2CH2Cl
CON 2 hours, room temperature

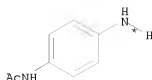
RX(137) OF 342 COMPOSED OF RX(57), RX(73)
RX(137) CR + CQ + DS ==> EO



CR

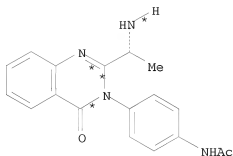


CQ



DS

2
STEPS
→



EO
YIELD 90%

RX(57) RCT CR 118-92-3, CQ 7764-95-6

STAGE(1)

RGT U 110-86-1 Pyridine, CZ 101-02-0 P(OPh)3
CON 3 hours, 70 deg C

STAGE(2)

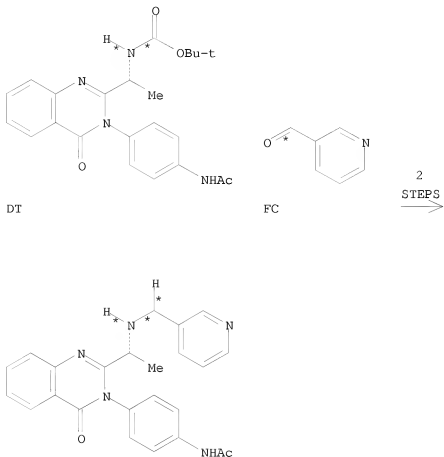
RCT DS 122-80-5
CON 1 hour, 55 deg C

PRO DT 944915-41-7

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RX(73) RCT DT 944915-41-7
 RGT ED 76-05-1 F3CCO2H
 PRO EO 944915-56-4
 SOL 75-09-2 CH2Cl2
 CON 2 hours, room temperature

RX(163) OF 342 COMPOSED OF RX(73), RX(98)
 RX(163) DT + FC ==> BV

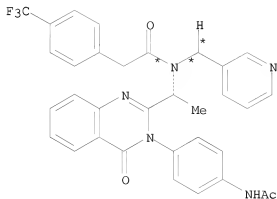
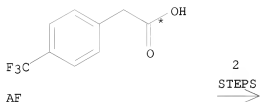
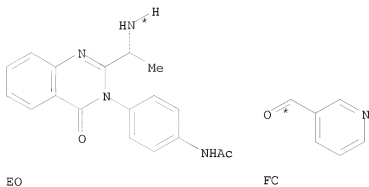


BV
 YIELD 80%

RX(73) RCT DT 944915-41-7
 RGT ED 76-05-1 F3CCO2H
 PRO EO 944915-56-4
 SOL 75-09-2 CH2Cl2
 CON 2 hours, room temperature

RX(98) RCT EO 944915-56-4, FC 500-22-1
 RGT O 56553-60-7 Na.(AcO)3BH
 PRO BV 944915-81-5
 SOL 107-06-2 ClCH2CH2Cl
 CON 2 hours, room temperature

RX(202) OF 342 COMPOSED OF RX(98), RX(34)
 RX(202) EO + FC + AF ==> BW



YIELD 90%

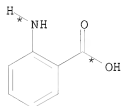
RX(98) RCT EO 944915-56-4, FC 500-22-1
 RGT O 56553-60-7 Na.(AcO)3BH
 PRO BV 944915-81-5
 SOL 107-06-2 ClCH2CH2Cl
 CON 2 hours, room temperature

RX(34) RCT BV 944915-81-5, AF 32857-62-8
 RGT D 2592-95-2 1-Benzotriazolol, E 25952-53-8 EDAP

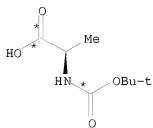
10/ 562,112

PRO BW 944915-21-3
SOL 68-12-2 DMF
CON 1 hour, room temperature

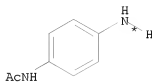
RX(246) OF 342 COMPOSED OF RX(57), RX(73), RX(98)
RX(246) CR + CQ + DS + FC ==> BV



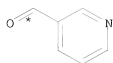
CR



CQ

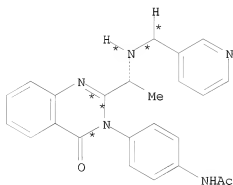


DS



FC

3
STEPS
→



BV
YIELD 80%

RX(57) RCT CR 118-92-3, CQ 7764-95-6

STAGE(1)

RGT U 110-86-1 Pyridine, CZ 101-02-0 P(OPh)₃
CON 3 hours, 70 deg C

STAGE(2)

RCT DS 122-80-5
CON 1 hour, 55 deg C

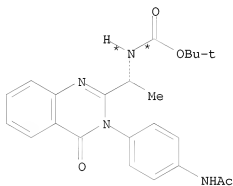
10/ 562,112

PRO DT 944915-41-7

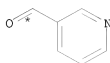
RX(73) RCT DT 944915-41-7
RGT ED 76-05-1 F3CCO2H
PRO EO 944915-56-4
SOL 75-09-2 CH2Cl2
CON 2 hours, room temperature

RX(98) RCT EO 944915-56-4, FC 500-22-1
RGT O 56553-60-7 Na.(AcO)3BH
PRO BV 944915-81-5
SOL 107-06-2 ClCH2CH2Cl
CON 2 hours, room temperature

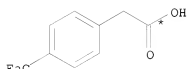
RX(321) OF 342 COMPOSED OF RX(73), RX(98), RX(34)
RX(321) DT + FC + AF ==> BW



DT

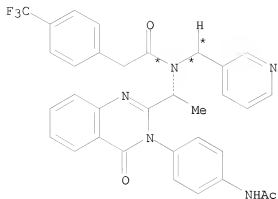


FC



AF

3
STEPS
=>



BW

YIELD 90%

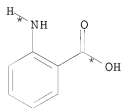
RX(73) RCT DT 944915-41-7
 RGT ED 76-05-1 F3CCO2H
 PRO EO 944915-56-4
 SOL 75-09-2 CH2Cl2
 CON 2 hours, room temperature

RX(98) RCT EO 944915-56-4, FC 500-22-1
 RGT O 56553-60-7 Na.(AcO)3BH
 PRO BV 944915-81-5
 SOL 107-06-2 ClCH2CH2Cl
 CON 2 hours, room temperature

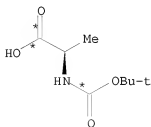
RX(34) RCT BV 944915-81-5, AF 32857-62-8
 RGT D 2592-95-2 1-Benzotriazolol, E 25952-53-8 EDAP
 PRO BW 944915-21-3
 SOL 68-12-2 DMF
 CON 1 hour, room temperature

RX(322) OF 342 COMPOSED OF RX(57), RX(73), RX(98), RX(34)

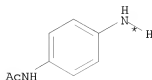
RX(322) CR + CQ + DS + FC + AF ==> BW



CR

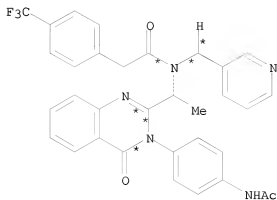
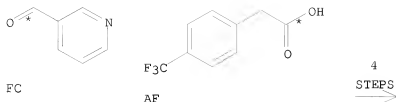


CQ



DS

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BW
YIELD 90%

RX(57) RCT CR 118-92-3, CQ 7764-95-6

STAGE(1)

RGT U 110-86-1 Pyridine, CZ 101-02-0 P(OPh)₃

CON 3 hours, 70 deg C

STAGE(2)

RCT DS 122-80-5

CON 1 hour, 55 deg C

PRO DT 944915-41-7

RX(73) RCT DT 944915-41-7
RGT ED 76-05-1 F3CCO₂H
PRO EO 944915-56-4
SOL 75-09-2 CH₂Cl₂
CON 2 hours, room temperature

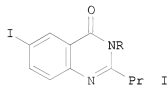
RX(98) RCT EO 944915-56-4, FC 500-22-1
RGT O 56553-60-7 Na.(AcO)3BH
PRO BV 944915-81-5
SOL 107-06-2 ClCH₂CH₂Cl
CON 2 hours, room temperature

RX(34) RCT BV 944915-81-5, AF 32857-62-8
RGT D 2592-95-2 1-Benzotriazolol, E 25952-53-8 EDAP
PRO BW 944915-21-3
SOL 68-12-2 DMF

CON 1 hour, room temperature

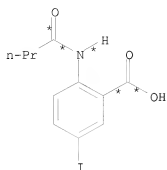
REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 19 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 147:211821 CASREACT
 TITLE: Synthesis of some new 4-(3H)-quinazoline analogs as potential antioxidant agents
 AUTHOR(S): Al-Omar, M. A.; El-Azab, Adel E.; El-Obeid, H. A.; Abdel Hamide, S. G.
 CORPORATE SOURCE: Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, Riyadh, 11451, Saudi Arabia
 SOURCE: Journal of Saudi Chemical Society (2006), 10(1), 113-128
 CODEN: JSCSFO; ISSN: 1319-6103
 PUBLISHER: Saudi Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB A new series of derivs. of 6-iodo-2-propyl-4(3H)-quinazolinone [I, R = H] and its fused heterocyclic analogs were prepared and screened for their antioxidant activity. I [R = H, NHCONH₂, OH, phthalimido, NH₂, O₂CCH₂Cl, OCH₂CONH₂] inhibit aldehyde oxidase exclusively by more than 98 %. This type of inhibition was found to be competitive with K_i value ranging from 50-400 μM with respect to aldehyde oxidase.

RX(32) OF 118 COMPOSED OF RX(2), RX(4)
 RX(32) C + J ==> K

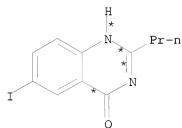


C



J

2
STEPS
→



K

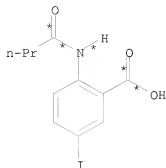
YIELD 70%

RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

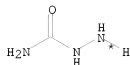
RX(4) RCT E 944830-81-3, J 75-12-7
PRO K 145863-89-4
SOL 75-12-7 Formamide
CON 2 hours, reflux

RX(33) OF 118 COMPOSED OF RX(2), RX(5)
RX(33) C + L ==> M

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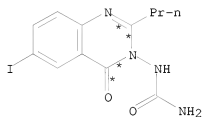


C



L

2
STEPS
→



M

YIELD 85%

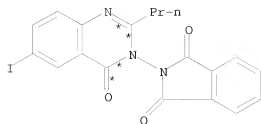
RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(5) RCT E 944830-81-3, L 57-56-7
PRO M 944830-83-5
SOL 110-86-1 Pyridine
CON 6 hours, reflux

RX(34) OF 118 COMPOSED OF RX(2), RX(7)

RX(34) C ==> Q

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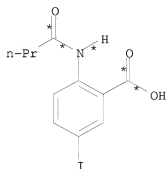


V
YIELD 72%

RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

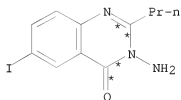
RX(9) RCT E 944830-81-3, U 1875-48-5
PRO V 944830-87-9
SOL 110-86-1 Pyridine
CON 6 - 12 hours, reflux

RX(37) OF 118 COMPOSED OF RX(2), RX(10)
RX(37) C ==> W



C

2
STEPS
→



W
YIELD 77%

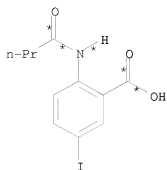
RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(10) RCT E 944830-81-3
RGT X 7803-57-8 N2H4-H2O
PRO W 944830-88-0
CON 1 hour, heated

RX(38) OF 118 COMPOSED OF RX(2), RX(11)

10/ 562,112

RX(38) C + Y ==> Z

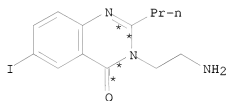


C



Y

2
STEPS
→



Z

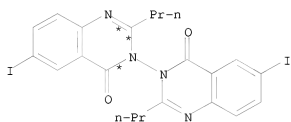
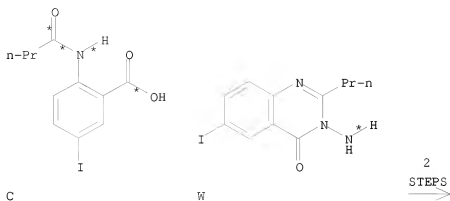
YIELD 45%

RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(11) RCT E 944830-81-3, Y 107-15-3
PRO Z 944830-89-1
SOL 64-17-5 EtOH
CON 2 hours, reflux

RX(39) OF 118 COMPOSED OF RX(2), RX(12)

RX(39) C + W ==> AB



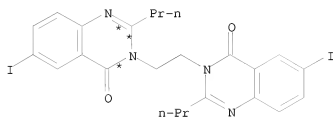
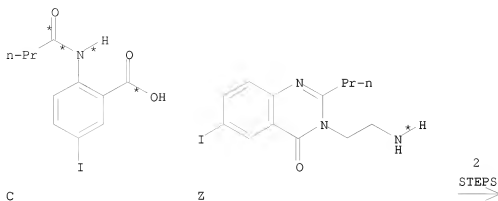
YIELD 63%

RX(2) RCT C 73721-77-4
 PRO E 944830-81-3
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(12) RCT E 944830-81-3, W 944830-88-0
 RGT O 127-09-3 AcONa
 PRO AB 944830-90-4
 SOL 64-19-7 AcOH
 CON 18 hours, reflux

RX(40) OF 118 COMPOSED OF RX(2), RX(13)
 RX(40) C + Z ==> AC

10/ 562,112

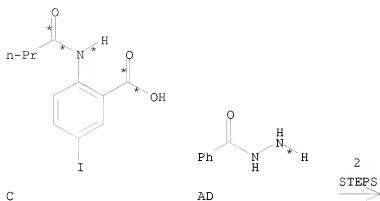


AC
YIELD 56%

RX(2) RCT C 73721-77-4
 PRO E 944830-81-3
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(13) RCT E 944830-81-3, Z 944830-89-1
 RGT O 127-09-3 AcONa
 PRO AC 944830-91-5
 SOL 64-19-7 AcOH
 CON 18 hours, reflux

RX(41) OF 118 COMPOSED OF RX(2), RX(14)
 RX(41) C + AD ==> AE

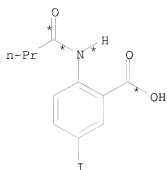


AE
YIELD 73%

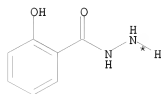
RX(2) RCT C 73721-77-4
 PRO E 944830-81-3
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(14) RCT E 944830-81-3, AD 613-94-5
 PRO AE 944830-93-7
 SOL 110-86-1 Pyridine
 CON 10 hours, reflux
 NIE alternative preparation shown

RX(42) OF 118 COMPOSED OF RX(2), RX(15)
 RX(42) C + AF ==> AG

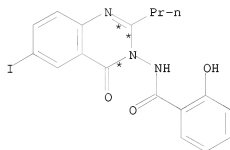


C



AF

2
STEPS
→



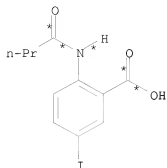
AG

YIELD 71%

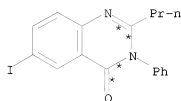
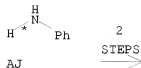
RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(15) RCT E 944830-81-3, AF 936-02-7
PRO AG 944830-94-8
SOL 110-86-1 Pyridine
CON 10 hours, reflux

RX(43) OF 118 COMPOSED OF RX(2), RX(17)
RX(43) C + AJ ==> AK



C



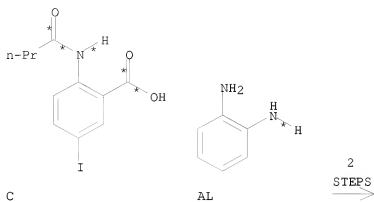
AK

YIELD 76%

RX(2) RCT C 73721-77-4
 PRO E 944830-81-3
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(17) RCT E 944830-81-3, AJ 62-53-3
 PRO AK 944830-96-0
 SOL 110-86-1 Pyridine
 CON 6 - 12 hours, reflux

RX(44) OF 118 COMPOSED OF RX(2), RX(18)
 RX(44) C + AL ==> AM



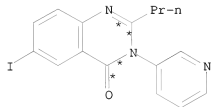
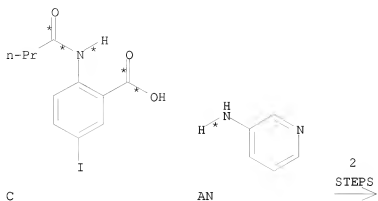
AM
YIELD 80%

RX(2) RCT C 73721-77-4
 PRO E 944830-81-3
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(18) RCT E 944830-81-3, AL 95-54-5
 PRO AM 944830-97-1
 SOL 110-86-1 Pyridine
 CON 6 - 12 hours, reflux

RX(45) OF 118 COMPOSED OF RX(2), RX(19)
 RX(45) C + AN ==> AO

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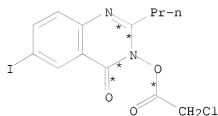
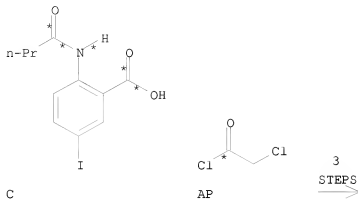


AO
YIELD 83%

RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(19) RCT E 944830-81-3, AN 462-08-8
PRO AO 944830-98-2
SOL 110-86-1 Pyridine
CON 6 - 12 hours, reflux

RX(76) OF 118 COMPOSED OF RX(2), RX(7), RX(20)
RX(76) C + AP ==> AQ

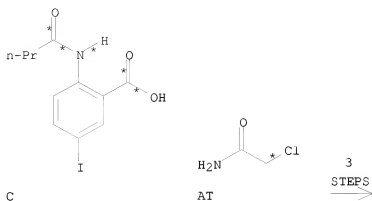


AQ

YIELD 80%

RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(7)	RCT	E 944830-81-3
	RGT	R 5470-11-1 H2NOH-HCl
	PRO	Q 944830-85-7
	SOL	110-86-1 Pyridine
	CON	6 - 12 hours, reflux
RX(20)	RCT	Q 944830-85-7, AP 79-04-9
	PRO	AQ 944830-99-3
	SOL	68-12-2 DMF
	CON	6 hours, reflux

RX(77) OF 118 COMPOSED OF RX(2), RX(7), RX(22)
 RX(77) C + AT ==> AU

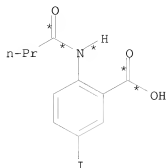


RX(2) RCT C 73721-77-4
 PRO E 944830-81-3
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

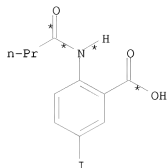
RX(7) RCT E 944830-81-3
 RGT R 5470-11-1 H2NOH-HCl
 PRO Q 944830-85-7
 SOL 110-86-1 Pyridine
 CON 6 - 12 hours, reflux

RX(22) RCT Q 944830-85-7, AT 79-07-2
 PRO AU 944831-01-0
 SOL 68-12-2 DMF
 CON 6 hours, reflux

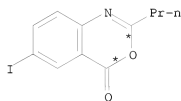
RX(78) OF 118 COMPOSED OF RX(2), RX(10), RX(12)
 RX(78) 2 C + E ==> AB



C

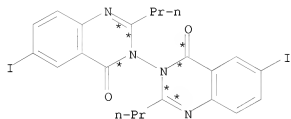


C



E

3
STEPS
→



AB

YIELD 63%

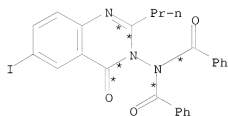
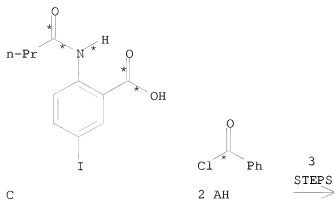
RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(10)	RCT	E 944830-81-3
	RGT	X 7803-57-8 N2H4-H2O
	PRO	W 944830-88-0
	CON	1 hour, heated
RX(12)	RCT	E 944830-81-3, W 944830-88-0
	RGT	O 127-09-3 AcONa
	PRO	AB 944830-90-4
	SOL	64-19-7 AcOH

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CON 18 hours, reflux

RX(79) OF 118 COMPOSED OF RX(2), RX(10), RX(16)

RX(79) C + 2 AH ==> AI



AI

YIELD 81%

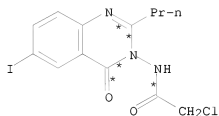
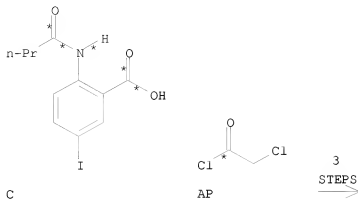
RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(10) RCT E 944830-81-3
RGT X 7803-57-8 N2H4-H2O
PRO W 944830-88-0
CON 1 hour, heated

RX(16) RCT W 944830-88-0, AH 98-88-4
PRO AI 944830-95-9
SOL 110-86-1 Pyridine
CON 7 hours, reflux

RX(80) OF 118 COMPOSED OF RX(2), RX(10), RX(21)

RX(80) C + AP ==> AS



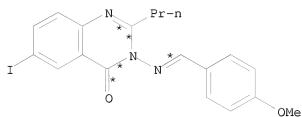
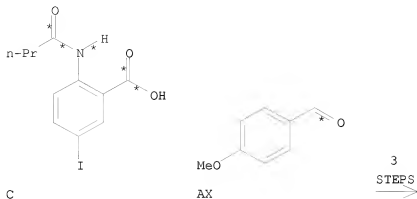
YIELD 71%

RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(10)	RCT	E 944830-81-3
	RGT	X 7803-57-8 N2H4-H2O
	PRO	W 944830-88-0
	CON	1 hour, heated
RX(21)	RCT	W 944830-88-0, AP 79-04-9
	PRO	AS 944831-00-9
	SOL	68-12-2 DMF
	CON	5 hours, room temperature

RX(81) OF 118 COMPOSED OF RX(2), RX(10), RX(24)

RX(81) C + AX ==> AY

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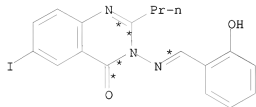
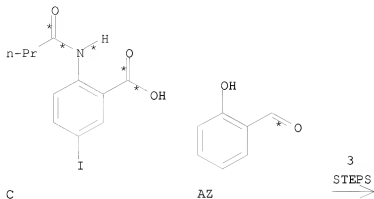
YIELD 79%

RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(10) RCT E 944830-81-3
RGT X 7803-57-8 N2H4-H2O
PRO W 944830-88-0
CON 1 hour, heated

RX(24) RCT W 944830-88-0, AX 123-11-5
PRO AY 944831-03-2
SOL 64-19-7 AcOH
CON 9 hours, reflux

RX(82) OF 118 COMPOSED OF RX(2), RX(10), RX(25)
RX(82) C + AZ ==> BA



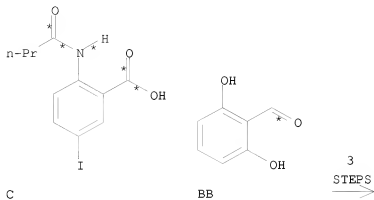
BA
YIELD 83%

RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(10) RCT E 944830-81-3
RGT X 7803-57-8 N2H4-H2O
PRO W 944830-88-0
CON 1 hour, heated

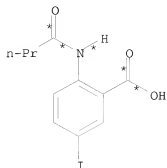
RX(25) RCT W 944830-88-0, AZ 90-02-8
PRO BA 944831-04-3
SOL 64-19-7 AcOH
CON 9 hours, reflux

RX(83) OF 118 COMPOSED OF RX(2), RX(10), RX(26)
RX(83) C + BB ==> BC

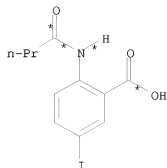


BC
YIELD 70%

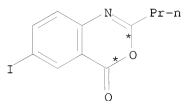
RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(10)	RCT	E 944830-81-3
	RGT	X 7803-57-8 N2H4-H2O
	PRO	W 944830-88-0
	CON	1 hour, heated
RX(26)	RCT	W 944830-88-0, BB 387-46-2
	PRO	BC 944831-05-4
	SOL	64-19-7 AcOH
	CON	9 hours, reflux
RX(84)	OF	118 COMPOSED OF RX(2), RX(11), RX(13)
RX(84)	2 C	+ Y + E ==> AC



C



C

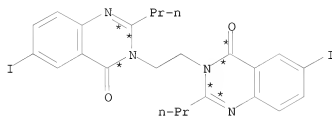


E



Y

3
STEPS
→



AC

YIELD 56%

RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(11)	RCT	E 944830-81-3, Y 107-15-3
	PRO	Z 944830-89-1
	SOL	64-17-5 EtOH
	CON	2 hours, reflux
RX(13)	RCT	E 944830-81-3, Z 944830-89-1
	RGT	O 127-09-3 AcONa
	PRO	AC 944830-91-5
	SOL	64-19-7 AcOH

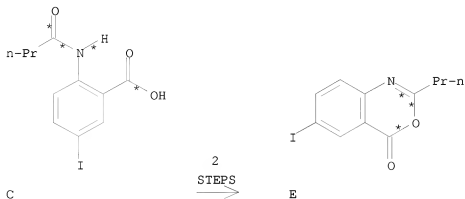
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CON 18 hours, reflux

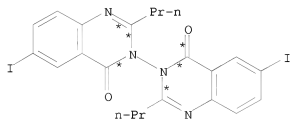
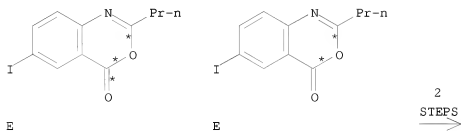
RX(97) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(12)
AND REACTION SEQUENCE RX(10), RX(12)

... C ==> E...

...2 E ==> AB



START NEXT REACTION SEQUENCE



YIELD 63%

RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(10) RCT E 944830-81-3
RGT X 7803-57-8 N2H4-H2O

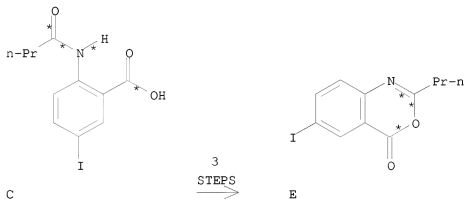
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PRO W 944830-88-0
CON 1 hour, heated

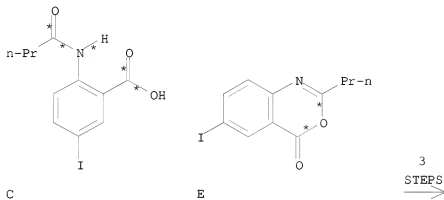
RX(12) RCT E 944830-81-3, W 944830-88-0
RGT O 127-09-3 AcONa
PRO AB 944830-90-4
SOL 64-19-7 AcOH
CON 18 hours, reflux

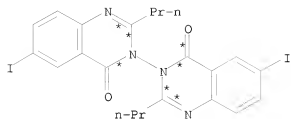
RX(101) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(12)
AND REACTION SEQUENCE RX(2), RX(10), RX(12)

... C ==> E...
... C + E ==> AB



START NEXT REACTION SEQUENCE





AB

YIELD 63%

RX(2) RCT C 73721-77-4
 PRO E 944830-81-3
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

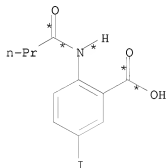
RX(2) RCT C 73721-77-4
 PRO E 944830-81-3
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(10) RCT E 944830-81-3
 RGT X 7803-57-8 N2H4-H2O
 PRO W 944830-88-0
 CON 1 hour, heated

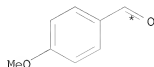
RX(12) RCT E 944830-81-3, W 944830-88-0
 RGT O 127-09-3 AcONa
 PRO AB 944830-90-4
 SOL 64-19-7 AcOH
 CON 18 hours, reflux

RX(102) OF 118 COMPOSED OF RX(2), RX(10), RX(24), RX(27)

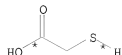
RX(102) C + AX + BD ==> BE



C



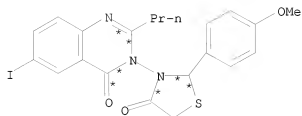
AX



BD

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4
STEPS
→



BE
YIELD 60%

RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(10) RCT E 944830-81-3
RGT X 7803-57-8 N2H4-H2O
PRO W 944830-88-0
CON 1 hour, heated

RX(24) RCT W 944830-88-0, AX 123-11-5
PRO AY 944831-03-2
SOL 64-19-7 AcOH
CON 9 hours, reflux

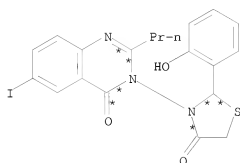
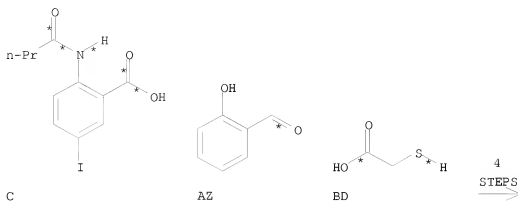
RX(27) RCT AY 944831-03-2, BD 68-11-1

STAGE(1)
SOL 71-43-2 Benzene
CON 12 hours, reflux

STAGE(2)
RGT BF 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON neutralized

PRO BE 944831-06-5

RX(103) OF 118 COMPOSED OF RX(2), RX(10), RX(25), RX(28)
RX(103) C + AZ + BD ==> BH



BH
YIELD 55%

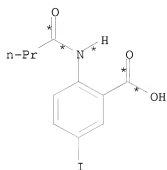
RX(2)	RCT C 73721-77-4
	PRO E 944830-81-3
	SOL 108-24-7 Ac2O
	CON 4 hours, reflux
RX(10)	RCT E 944830-81-3
	RGT X 7803-57-8 N2H4-H2O
	PRO W 944830-88-0
	CON 1 hour, heated
RX(25)	RCT W 944830-88-0, AZ 90-02-8
	PRO BA 944831-04-3
	SOL 64-19-7 AcOH
	CON 9 hours, reflux
RX(28)	RCT BA 944831-04-3, BD 68-11-1
	STAGE(1)
	SOL 71-43-2 Benzene
	CON 12 hours, reflux
	STAGE(2)
	RGT BF 497-19-8 Na2CO3
	SOL 7732-18-5 Water

CON neutralized

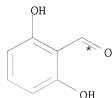
PRO BH 944831-07-6

RX(104) OF 118 COMPOSED OF RX(2), RX(10), RX(26), RX(29)

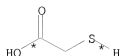
RX(104) C + BB + BD ==> BI



C

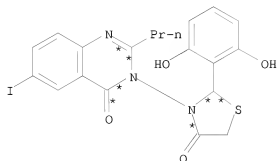


BB



BD

4
STEPS
→



BI
YIELD 51%

RX(2)	RCT C 73721-77-4
	PRO E 944830-81-3
	SOL 108-24-7 Ac2O
	CON 4 hours, reflux
RX(10)	RCT E 944830-81-3
	RGT X 7803-57-8 N2H4-H2O
	PRO W 944830-88-0
	CON 1 hour, heated
RX(26)	RCT W 944830-88-0, BB 387-46-2
	PRO BC 944831-05-4
	SOL 64-19-7 AcOH
	CON 9 hours, reflux
RX(29)	RCT BC 944831-05-4, BD 68-11-1

STAGE(1)

SOL 71-43-2 Benzene
CON 12 hours, reflux

STAGE(2)

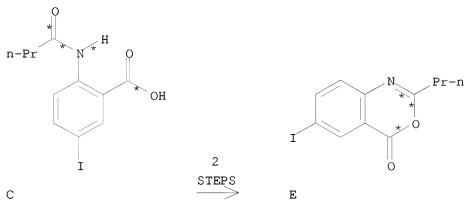
RGT BF 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON neutralized

PRO BI 944831-08-7

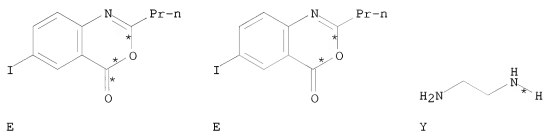
RX(105) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(13)
AND REACTION SEQUENCE RX(11), RX(13)

... C ==> E...

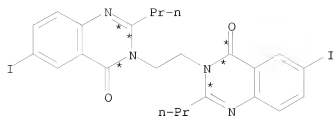
...2 E + Y ==> AC



START NEXT REACTION SEQUENCE



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AC
YIELD 56%

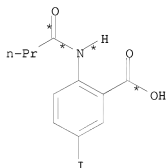
RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(11) RCT E 944830-81-3, Y 107-15-3
PRO Z 944830-89-1
SOL 64-17-5 EtOH
CON 2 hours, reflux

RX(13) RCT E 944830-81-3, Z 944830-89-1
RGT O 127-09-3 AcONa
PRO AC 944830-91-5
SOL 64-19-7 AcOH
CON 18 hours, reflux

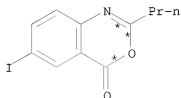
RX(106) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(13)
AND REACTION SEQUENCE RX(2), RX(11), RX(13)

... C ==> E...
... C + Y + E ==> AC



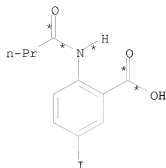
C

3
STEPS
→

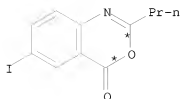


E

START NEXT REACTION SEQUENCE



C

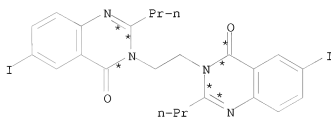


E



Y

3
STEPS
→

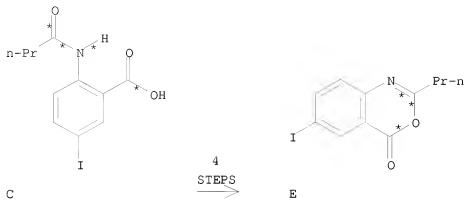


AC
YIELD 56%

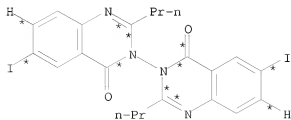
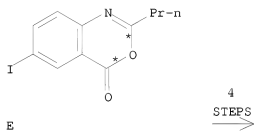
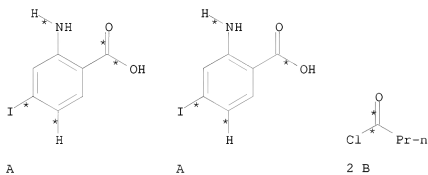
RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(2)	RCT	C 73721-77-4
	PRO	E 944830-81-3
	SOL	108-24-7 Ac2O
	CON	4 hours, reflux
RX(11)	RCT	E 944830-81-3, Y 107-15-3
	PRO	Z 944830-89-1
	SOL	64-17-5 EtOH
	CON	2 hours, reflux
RX(13)	RCT	E 944830-81-3, Z 944830-89-1
	RGT	O 127-09-3 AcONa
	PRO	AC 944830-91-5
	SOL	64-19-7 AcOH
	CON	18 hours, reflux

RX(109) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(12)
AND REACTION SEQUENCE RX(1), RX(2), RX(10), RX(12)

... C ==> E...
...2 A + 2 B + E ==> AB



START NEXT REACTION SEQUENCE



YIELD 63%

RX(2) RCT C 73721-77-4
 PRO E 944830-81-3
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

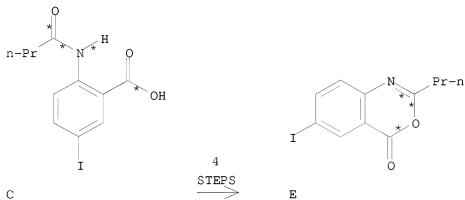
 RX(1) RCT A 20776-54-9, B 141-75-3
 PRO C 73721-77-4
 SOL 110-86-1 Pyridine
 CON 2 hours, room temperature

 RX(2) RCT C 73721-77-4
 PRO E 944830-81-3
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

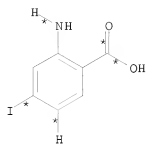
 RX(10) RCT E 944830-81-3
 RGT X 7803-57-8 N2H4-H2O
 PRO W 944830-88-0
 CON 1 hour, heated

 RX(12) RCT E 944830-81-3, W 944830-88-0
 RGT O 127-09-3 AcONa
 PRO AB 944830-90-4
 SOL 64-19-7 AcOH
 CON 18 hours, reflux

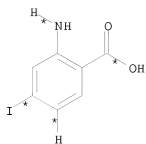
RX(114) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(13)
 AND REACTION SEQUENCE RX(1), RX(2), RX(11), RX(13)
 ... C ==> E...
 ...2 A + 2 B + Y + E ==> AC



START NEXT REACTION SEQUENCE



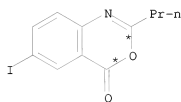
A



A



2 B

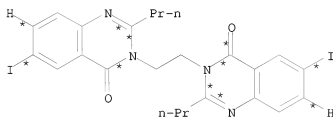


E



Y

4
STEPS
→



AC

YIELD 56%

RX(2)	RCT C 73721-77-4
	PRO E 944830-81-3
	SOL 108-24-7 Ac2O
	CON 4 hours, reflux
RX(1)	RCT A 20776-54-9, B 141-75-3
	PRO C 73721-77-4
	SOL 110-86-1 Pyridine
	CON 2 hours, room temperature
RX(2)	RCT C 73721-77-4
	PRO E 944830-81-3
	SOL 108-24-7 Ac2O
	CON 4 hours, reflux
RX(11)	RCT E 944830-81-3, Y 107-15-3
	PRO Z 944830-89-1

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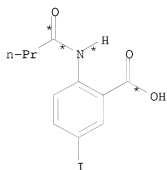
SOL 64-17-5 EtOH
CON 2 hours, reflux

RX(13) RCT E 944830-81-3, Z 944830-89-1
RGT O 127-09-3 AcONa
PRO AC 944830-91-5
SOL 64-19-7 AcOH
CON 18 hours, reflux

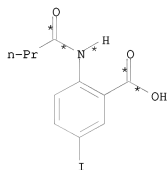
RX(115) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(10), RX(12)
AND REACTION SEQUENCE RX(1), RX(2), RX(12)

...2 C ==> W...

...A + B + W ==> AB

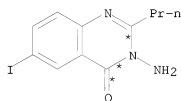


C



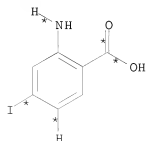
C

3
STEPS
→



W

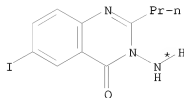
START NEXT REACTION SEQUENCE



A

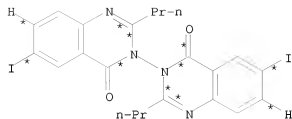


B



W

3
STEPS
→



AB
YIELD 63%

```

RX(2)      RCT  C 73721-77-4
           PRO  E 944830-81-3
           SOL  108-24-7 Ac2O
           CON  4 hours, reflux

RX(10)     RCT  E 944830-81-3
           RGT  X 7803-57-8 N2H4-H2O
           PRO  W 944830-88-0
           CON  1 hour, heated

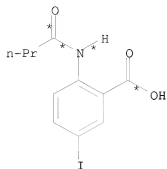
RX(1)      RCT  A 20776-54-9, B 141-75-3
           PRO  C 73721-77-4
           SOL  110-86-1 Pyridine
           CON  2 hours, room temperature

RX(2)      RCT  C 73721-77-4
           PRO  E 944830-81-3
           SOL  108-24-7 Ac2O
           CON  4 hours, reflux

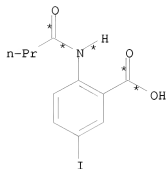
RX(12)     RCT  E 944830-81-3, W 944830-88-0
           RGT  O 127-09-3 AcONa
           PRO  AB 944830-90-4
           SOL  64-19-7 AcOH
           CON  18 hours, reflux

RX(116) OF 118 COMPOSED OF REACTION SEQUENCE RX(2), RX(11), RX(13)
           AND REACTION SEQUENCE RX(1), RX(2), RX(13)
...2 C + Y ==> Z...
...A + B + Z ==> AC

```



C

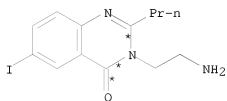


C



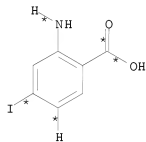
Y

3
STEPS
→



Z

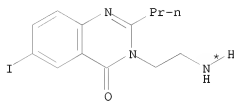
START NEXT REACTION SEQUENCE



A

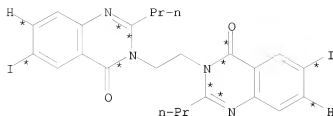


B



Z

3
STEPS
→



AC
YIELD 56%

RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(11) RCT E 944830-81-3, Y 107-15-3
PRO Z 944830-89-1
SOL 64-17-5 EtOH
CON 2 hours, reflux

RX(1) RCT A 20776-54-9, B 141-75-3
PRO C 73721-77-4
SOL 110-86-1 Pyridine
CON 2 hours, room temperature

RX(2) RCT C 73721-77-4
PRO E 944830-81-3
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(13) RCT E 944830-81-3, Z 944830-89-1
RGT O 127-09-3 AcONa
PRO AC 944830-91-5
SOL 64-19-7 AcOH
CON 18 hours, reflux

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

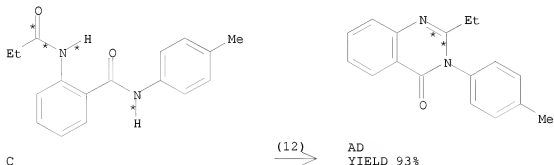
L3 ANSWER 20 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 147:52862 CASREACT
TITLE: Hexamethyldisilazane-iodine induced intramolecular
dehydrative cyclization of diamides: A general access
to natural and unnatural quinoxalinones
AUTHOR(S): Kshirsagar, Umesh A.; Mhaske, Santosh B.; Argade,
Narshinha P.
CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National
Chemical Laboratory, Pune, 411 008, India
SOURCE: Tetrahedron Letters (2007), 48(18), 3243-3246
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal

LANGUAGE:

English

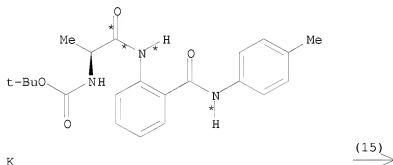
AB A simple and efficient general approach to various quinazolinone scaffolds, including peptidomimetic examples, has been demonstrated by employing hexamethyldisilazane-iodine-induced intramol. dehydrative cyclization of diamides. The N-protecting groups, such as Boc, Fmoc and Cbz, are tolerated and no racemization of optically active substrates was observed. The present protocol has also been used as a key step for the efficient four-step syntheses of the naturally occurring quinazolinones, such as sclerotigenin, (-)-circumdatin-F and (-)-fumiquinazoline-F.

RX(12) OF 45 ...C ==> AD

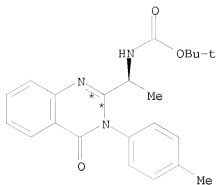


RX(12) RCT C 25628-87-9
 RGT AE 999-97-3 (Me3Si)2NH, AF 7553-56-2 I2
 PRO AD 50498-61-8
 SOL 75-09-2 CH2Cl2
 CON 30 minutes, room temperature

RX(15) OF 45 ...K ==> AI



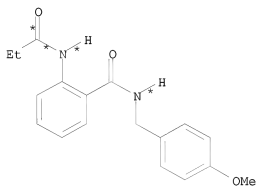
10/ 562,112



AI
YIELD 70%

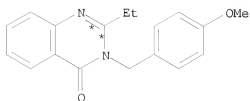
RX(15) RCT K 939966-28-6
RGT AE 999-97-3 (Me3Si)2NH, AF 7553-56-2 I2
PRO AI 939966-46-8
SOL 75-09-2 CH2Cl2
CON 4 hours, room temperature

RX(16) OF 45 ...O ==> AJ



O

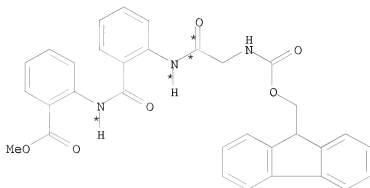
(16) →



AJ
YIELD 97%

RX(16) RCT O 939966-30-0
 RGT AE 999-97-3 (Me3Si)2NH, AF 7553-56-2 I2
 PRO AJ 939966-48-0
 SOL 75-09-2 CH2Cl2
 CON 3 hours, room temperature

RX(19) OF 45 ...U ==> AM...



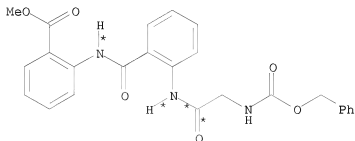
U

(19) →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(19) RCT U 939966-36-6
 RGT AE 999-97-3 (Me3Si)2NH, AF 7553-56-2 I2
 PRO AM 939966-54-8
 SOL 75-09-2 CH2Cl2
 CON 4 hours, room temperature

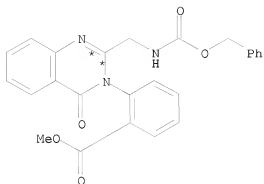
RX(20) OF 45 ...Y ==> AN...



Y

(20) →

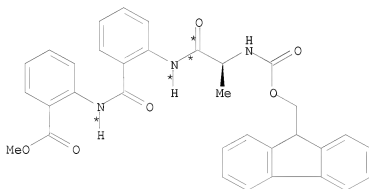
10/ 562,112



AN
YIELD 65%

RX(20) RCT Y 939966-38-8
RGT AE 999-97-3 (Me3Si)2NH, AF 7553-56-2 I2
PRO AN 939966-56-0
SOL 75-09-2 CH2Cl2
CON 4 hours, room temperature

RX(21) OF 45 ...AA ==> AO...



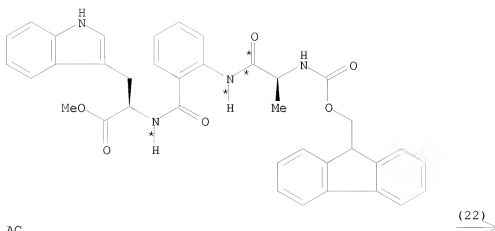
AA

(21) →

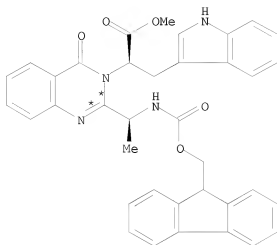
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(21) RCT AA 939966-40-2
RGT AE 999-97-3 (Me3Si)2NH, AF 7553-56-2 I2
PRO AO 939966-58-2
SOL 71-43-2 Benzene
CON 4 hours, reflux

RX(22) OF 45 ...AC ==> AQ...



AC



AQ

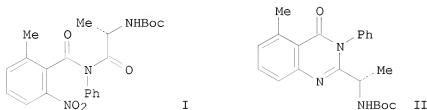
YIELD 65%

RX(22) RCT AC 262590-35-2
 RGT AE 999-97-3 (Me3Si)2NH, AF 7553-56-2 I2
 PRO AQ 939966-60-6
 SOL 71-43-2 Benzene
 CON 3 hours, reflux

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

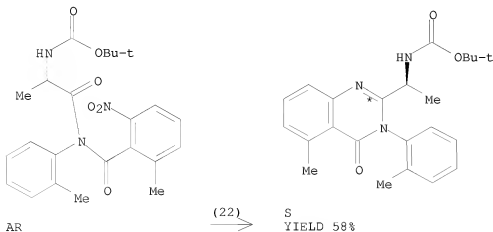
L3 ANSWER 21 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 146:500996 CASREACT
 TITLE: A Novel Highly Stereoselective Synthesis of
 2,3-Disubstituted 3H-Quinazoline-4-one Derivatives
 AUTHOR(S): Zhichkin, Paul; Kesicki, Edward; Treiberg, Jennifer;

Bourdon, Lisa; Ronsheim, Matthew; Ooi, Hua Chee;
 White, Stephen; Judkins, Angela; Fairfax, David
 CORPORATE SOURCE: Albany Molecular Research, Inc., Albany, NY, 12212,
 USA
 SOURCE: Organic Letters (2007), 9(7), 1415-1418
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB An efficient three-step synthesis of chiral 3H-quinazolin-4-one derivs.
 from com. materials is disclosed. The Mumm reaction of nitrobenzimidoyl
 chlorides with chiral L- α -amino acids, which were prepared by
 chlorination of nitrobenzamides, affords the corresponding
 (nitrobenzamido)oxoethylcarbamate derivs, e.g., I. Reductive
 cyclocondensation of the (nitrobenzamido)oxoethylcarbamate derivs affords
 enantiomerically pure (ee >93%) quinazolin-4-ones, e.g., II, in good
 overall yield. A comparison with existing approaches indicates that this
 method is superior for hindered substrates.

RX(22) OF 58 ...AR ==> S

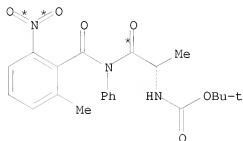


RX(22) RCT AR 936025-18-2
 RGT U 64-19-7 AcOH, BC 7440-66-6 Zn
 PRO S 936024-96-3
 SOL 64-19-7 AcOH
 CON SUBSTAGE(1) 20 deg C

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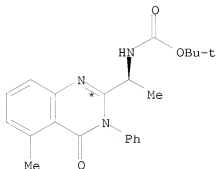
SUBSTAGE(2) 3.5 hours, room temperature
NTE alternative preparation shown, optimized on reducing agents,
>99% ee, optimization study

RX(23) OF 58 ...AS ==> BD



AS

(23) →

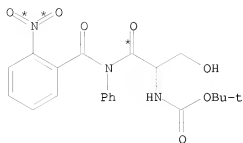


BD
YIELD 60%

RX(23) RCT AS 936025-19-3
RGT U 64-19-7 AcOH, BC 7440-66-6 Zn
PRO BD 936025-30-8
SOL 64-19-7 AcOH
CON SUBSTAGE(1) 1 hour, room temperature
SUBSTAGE(2) 3 hours, room temperature
SUBSTAGE(3) room temperature
NTE 98% ee, incremental addition of Zn

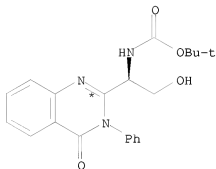
RX(26) OF 58 ...AZ ==> BG

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AZ

(26)

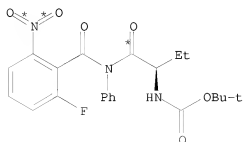


BG

YIELD 57%

RX(26) RCT AZ 936025-27-3
 RGT U 64-19-7 AcOH, BC 7440-66-6 Zn
 PRO BG 936025-35-3
 SOL 64-19-7 AcOH
 CON 6 hours, room temperature
 NTE 94% ee

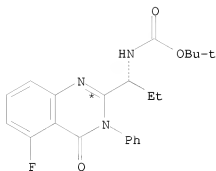
RX(27) OF 58 ...BB ==> BH



BB

(27)

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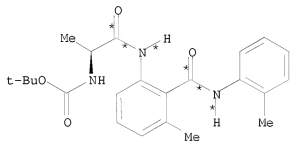
BH

YIELD 67%

RX(27) RCT BB 936025-29-5
 RGT U 64-19-7 AcOH, BC 7440-66-6 Zn
 PRO BH 936025-37-5
 SOL 64-19-7 AcOH
 CON SUBSTAGE(1) 15 minutes, >room temperature
 SUBSTAGE(2) 17.5 hours, room temperature
 NTE >98% ee, incremental addition of Zn

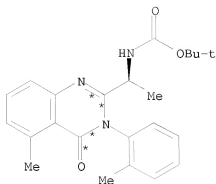
RX(33) OF 58 COMPOSED OF RX(3), RX(4)

RX(33) J ==> S



J

2
 STEPS
 →



S
YIELD 94%

RX(3)

STAGE(1)

RGT O 7726-95-6 Br2, P 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON 30 minutes, room temperature

STAGE(2)

RCT J 936024-93-0
RGT Q 121-44-8 Et3N
CON SUBSTAGE(1) reflux
SUBSTAGE(2) 1.5 hours, reflux

PRO N 936024-94-1
NTE stage 2 exothermic

RX(4) RCT N 936024-94-1

STAGE(1)

RGT T 123-75-1 Pyrrolidine
SOL 123-75-1 Pyrrolidine
CON overnight, room temperature

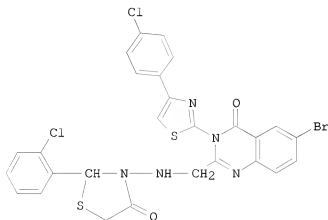
STAGE(2)

RGT U 64-19-7 AcOH
SOL 75-05-8 MeCN
CON 30 minutes, reflux

PRO S 936024-96-3
NTE alternative preparation shown, 96% ee, 14% overall yield for 3 steps

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

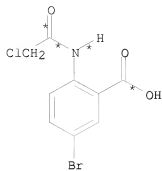
TITLE: Synthesis of 3-[4'-(p-chlorophenyl)-thiazol-2'-yl]-2-
[(substituted azetidinone/thiazolidinone)-aminomethyl]-
6-bromoquinazolin-4-ones as anti-inflammatory agent
AUTHOR(S): Kumar, Ashok; Rajput, Chatrasal Singh; Bhati, Sudhir
Kumar
CORPORATE SOURCE: Department of Pharmacology, L L R M Medical College,
Meerut (UP), 250004, India
SOURCE: Bioorganic & Medicinal Chemistry (2007), 15(8),
3089-3096
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



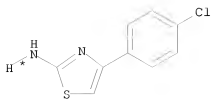
I

AB Title compds. were prepared and screened for anti-inflammatory and analgesic activities at the dose of 50 mg/kg po. Compound 21 (I) showed maximum anti-inflammatory (38.35%) and analgesic (37.36%) activities. Compound 21 was also tested for ulcerogenic activity and the UD50 value was found to be 195.6 mg/kg po.

RX(2) OF 118 ...C + F ==> G...

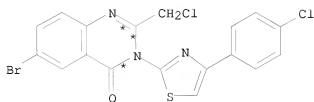


C



F

(2)

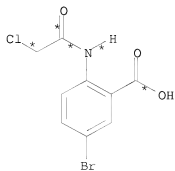


G

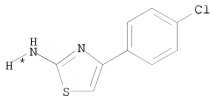
YIELD 55%

RX(2) RCT C 155104-20-4, F 2103-99-3
 RGT H 584-08-7 K₂CO₃
 PRO G 935702-18-4
 SOL 71-43-2 Benzene
 CON 2 hours, reflux

RX(29) OF 118 COMPOSED OF RX(2), RX(3)
 RX(29) C + F ==> I

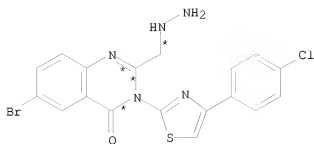


C



F

2
STEPS



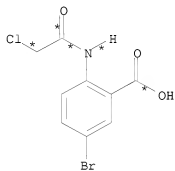
I
YIELD 62%

RX(2) RCT C 155104-20-4, F 2103-99-3
RGT H 584-08-7 K2CO3
PRO G 935702-18-4
SOL 71-43-2 Benzene
CON 2 hours, reflux

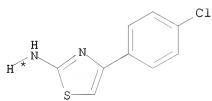
RX(3) RCT G 935702-18-4
RGT J 7803-57-8 N2H4-H2O
PRO I 935702-19-5
SOL 64-17-5 EtOH
CON 10 hours, reflux

RX(55) OF 118 COMPOSED OF RX(2), RX(3), RX(4)

RX(55) C + F + L ==> M



C

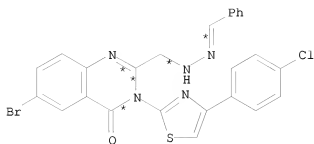


F



L

3
STEPS
→



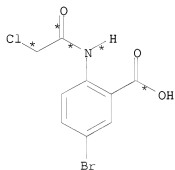
M
YIELD 65%

RX(2) RCT C 155104-20-4, F 2103-99-3
RGT H 584-08-7 K2CO3
PRO G 935702-18-4
SOL 71-43-2 Benzene
CON 2 hours, reflux

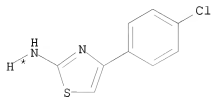
RX(3) RCT G 935702-18-4
RGT J 7803-57-8 N2H4-H2O
PRO I 935702-19-5
SOL 64-17-5 EtOH
CON 10 hours, reflux

RX(4) RCT I 935702-19-5, L 100-52-7
PRO M 935702-20-8
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON 8 hours, reflux

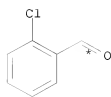
RX(56) OF 118 COMPOSED OF RX(2), RX(3), RX(5)
RX(56) C + F + O ==> P



C



F



O

3
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

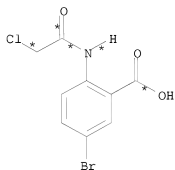
RX(2) RCT C 155104-20-4, F 2103-99-3
 RGT H 584-08-7 K₂CO₃
 PRO G 935702-18-4
 SOL 71-43-2 Benzene
 CON 2 hours, reflux

RX(3) RCT G 935702-18-4
 RGT J 7803-57-8 N₂H₄-H₂O
 PRO I 935702-19-5
 SOL 64-17-5 EtOH
 CON 10 hours, reflux

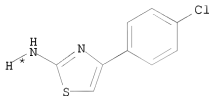
RX(5) RCT I 935702-19-5, O 89-98-5
 PRO P 935702-21-9
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON reflux

RX(57) OF 118 COMPOSED OF RX(2), RX(3), RX(6)

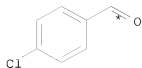
RX(57) C + F + Q ==> R



C

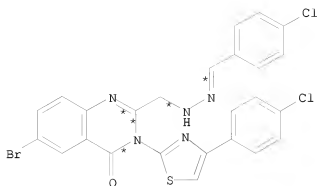


F



Q

3
 STEPS
 →



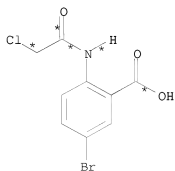
R
YIELD 58%

RX(2) RCT C 155104-20-4, F 2103-99-3
RGT H 584-08-7 K2CO3
PRO G 935702-18-4
SOL 71-43-2 Benzene
CON 2 hours, reflux

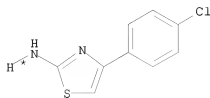
RX(3) RCT G 935702-18-4
RGT J 7803-57-8 N2H4-H2O
PRO I 935702-19-5
SOL 64-17-5 EtOH
CON 10 hours, reflux

RX(6) RCT I 935702-19-5, Q 104-88-1
PRO R 935702-22-0
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON reflux

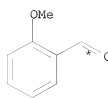
RX(58) OF 118 COMPOSED OF RX(2), RX(3), RX(7)
RX(58) C + F + S ==> T



C



F



S

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3
STEPS
→

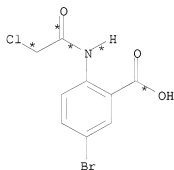
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 155104-20-4, F 2103-99-3
RGT H 584-08-7 K2CO3
PRO G 935702-18-4
SOL 71-43-2 Benzene
CON 2 hours, reflux

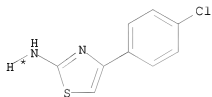
RX(3) RCT G 935702-18-4
RGT J 7803-57-8 N2H4-H2O
PRO I 935702-19-5
SOL 64-17-5 EtOH
CON 10 hours, reflux

RX(7) RCT I 935702-19-5, S 135-02-4
PRO T 935702-23-1
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON reflux

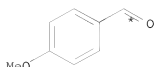
RX(59) OF 118 COMPOSED OF RX(2), RX(3), RX(8)
RX(59) C + F + U ==> V



C

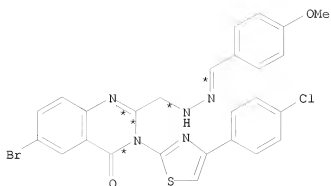


F



U

3
STEPS
→



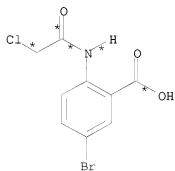
V
YIELD 60%

RX(2) RCT C 155104-20-4, F 2103-99-3
RGT H 584-08-7 K2CO3
PRO G 935702-18-4
SOL 71-43-2 Benzene
CON 2 hours, reflux

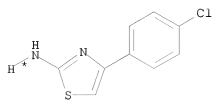
RX(3) RCT G 935702-18-4
RGT J 7803-57-8 N2H4-H2O
PRO I 935702-19-5
SOL 64-17-5 EtOH
CON 10 hours, reflux

RX(8) RCT I 935702-19-5, U 123-11-5
PRO V 935702-24-2
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON reflux

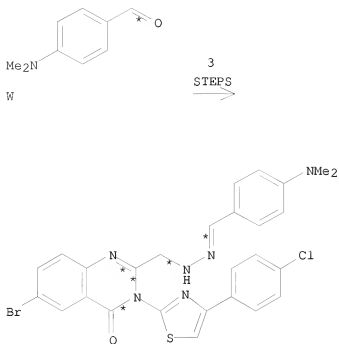
RX(60) OF 118 COMPOSED OF RX(2), RX(3), RX(9)
RX(60) C + F + W ==> X



C



F



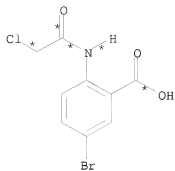
X
YIELD 65%

RX(2) RCT C 155104-20-4, F 2103-99-3
RGT H 584-08-7 K₂CO₃
PRO G 935702-18-4
SOL 71-43-2 Benzene
CON 2 hours, reflux

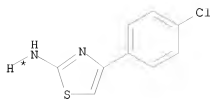
RX(3) RCT G 935702-18-4
RGT J 7803-57-8 N₂H₄-H₂O
PRO I 935702-19-5
SOL 64-17-5 EtOH
CON 10 hours, reflux

RX(9) RCT I 935702-19-5, W 100-10-7
PRO X 935702-25-3
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON reflux

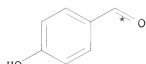
RX(61) OF 118 COMPOSED OF RX(2), RX(3), RX(10)
RX(61) C + F + Y ==> Z



C

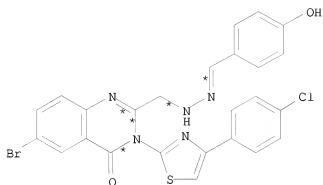


F



Y

3
STEPS
→



Z

YIELD 62%

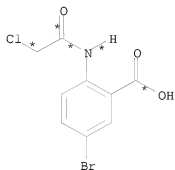
RX(2) RCT C 155104-20-4, F 2103-99-3
 RGT H 584-08-7 K₂CO₃
 PRO G 935702-18-4
 SOL 71-43-2 Benzene
 CON 2 hours, reflux

RX(3) RCT G 935702-18-4
 RGT J 7803-57-8 N₂H₄-H₂O
 PRO I 935702-19-5
 SOL 64-17-5 EtOH
 CON 10 hours, reflux

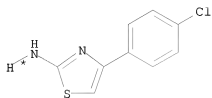
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RX(10) RCT I 935702-19-5, Y 123-08-0
PRO Z 935702-26-4
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON reflux

RX(62) OF 118 COMPOSED OF RX(2), RX(3), RX(11)
RX(62) C + F + AA ==> AB



C



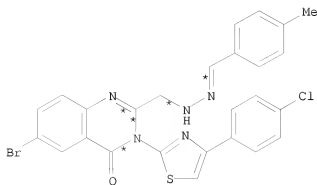
F



Me

AA

3
STEPS
→



AB

YIELD 59%

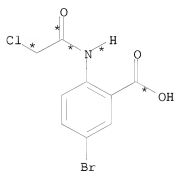
RX(2) RCT C 155104-20-4, F 2103-99-3

RGT H 584-08-7 K2CO3
 PRO G 935702-18-4
 SOL 71-43-2 Benzene
 CON 2 hours, reflux

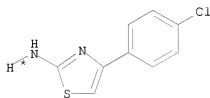
RX(3) RCT G 935702-18-4
 RGT J 7803-57-8 N2H4-H2O
 PRO I 935702-19-5
 SOL 64-17-5 EtOH
 CON 10 hours, reflux

RX(11) RCT I 935702-19-5, AA 104-87-0
 PRO AB 935702-27-5
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON reflux

RX(87) OF 118 COMPOSED OF RX(2), RX(3), RX(4), RX(12)
 RX(87) C + F + L + B ==> AC



C



F

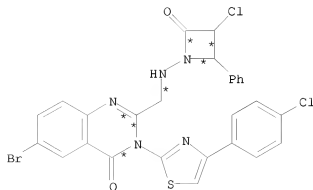


L



B

4
 STEPS
 →



AC
 YIELD 55%

RX(2) RCT C 155104-20-4, F 2103-99-3
 RGT H 584-08-7 K2CO3

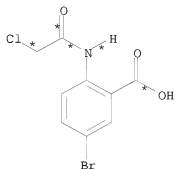
PRO G 935702-18-4
 SOL 71-43-2 Benzene
 CON 2 hours, reflux

RX(3) RCT G 935702-18-4
 RGT J 7803-57-8 N2H4-H2O
 PRO I 935702-19-5
 SOL 64-17-5 EtOH
 CON 10 hours, reflux

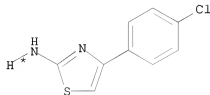
RX(4) RCT I 935702-19-5, L 100-52-7
 PRO M 935702-20-8
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 8 hours, reflux

RX(12) RCT M 935702-20-8, B 79-04-9
 RGT AD 121-44-8 Et3N
 PRO AC 935702-28-6
 SOL 71-43-2 Benzene
 CON SUBSTAGE(1) 50 deg C
 SUBSTAGE(2) 40 minutes, room temperature
 SUBSTAGE(3) 7 hours, reflux

RX(88) OF 118 COMPOSED OF RX(2), RX(3), RX(4), RX(20)
 RX(88) C + F + L + AL ==> AM



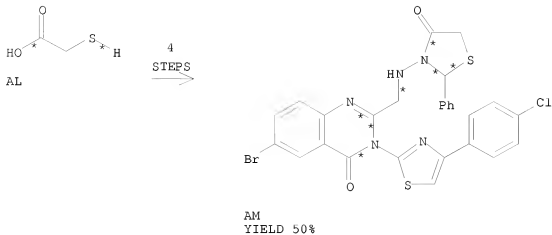
C



F



L



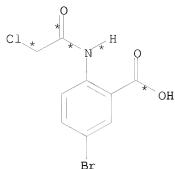
RX(2) RCT C 155104-20-4, F 2103-99-3
 RGT H 584-08-7 K₂CO₃
 PRO G 935702-18-4
 SOL 71-43-2 Benzene
 CON 2 hours, reflux

RX(3) RCT G 935702-18-4
 RGT J 7803-57-8 N₂H₄-H₂O
 PRO I 935702-19-5
 SOL 64-17-5 EtOH
 CON 10 hours, reflux

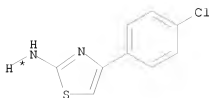
RX(4) RCT I 935702-19-5, L 100-52-7
 PRO M 935702-20-8
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON 8 hours, reflux

RX(20) RCT M 935702-20-8, AL 68-11-1
 PRO AM 935702-36-6
 CAT 7646-85-7 ZnCl₂
 SOL 71-43-2 Benzene
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 3 days, room temperature
 SUBSTAGE(3) 14 hours, reflux

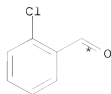
RX(89) OF 118 COMPOSED OF RX(2), RX(3), RX(5), RX(13)
 RX(89) C + F + O + B ==> AE



C



F



O



B

4
STEPS
➔

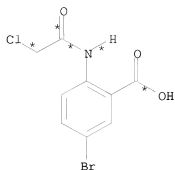
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2)	RCT	C 155104-20-4, F 2103-99-3
	RGT	H 584-08-7 K2CO3
	PRO	G 935702-18-4
	SOL	71-43-2 Benzene
	CON	2 hours, reflux
RX(3)	RCT	G 935702-18-4
	RGT	J 7803-57-8 N2H4-H2O
	PRO	I 935702-19-5
	SOL	64-17-5 EtOH
	CON	10 hours, reflux
RX(5)	RCT	I 935702-19-5, O 89-98-5
	PRO	P 935702-21-9
	CAT	64-19-7 AcOH
	SOL	64-17-5 EtOH
	CON	reflux
RX(13)	RCT	P 935702-21-9, B 79-04-9
	RGT	AD 121-44-8 Et3N
	PRO	AE 935702-29-7
	SOL	71-43-2 Benzene
	CON	SUBSTAGE(1) 50 deg C
		SUBSTAGE(2) room temperature
		SUBSTAGE(3) reflux

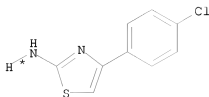
RX(90) OF 118 COMPOSED OF RX(2), RX(3), RX(5), RX(21)

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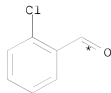
RX(90) C + F + O + AL ==> AO



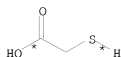
C



F



O



AL

4
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 155104-20-4, F 2103-99-3
RGT H 584-08-7 K2CO3
PRO G 935702-18-4
SOL 71-43-2 Benzene
CON 2 hours, reflux

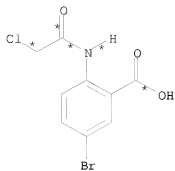
RX(3) RCT G 935702-18-4
RGT J 7803-57-8 N2H4-H2O
PRO I 935702-19-5
SOL 64-17-5 EtOH
CON 10 hours, reflux

RX(5) RCT I 935702-19-5, O 89-98-5
PRO P 935702-21-9
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON reflux

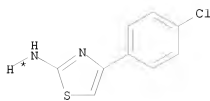
RX(21) RCT P 935702-21-9, AL 68-11-1
PRO AO 935702-37-7
CAT 7646-85-7 ZnCl2
SOL 71-43-2 Benzene
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) reflux

RX(91) OF 118 COMPOSED OF RX(2), RX(3), RX(6), RX(14)

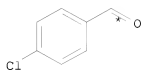
RX(91) C + F + Q + B ==> AF



C



F



Q



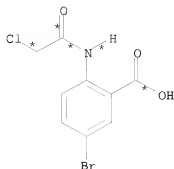
B

4
STEPS
→

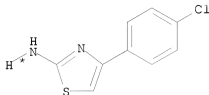
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2)	RCT	C 155104-20-4, F 2103-99-3
	RGT	H 584-08-7 K ₂ CO ₃
	PRO	G 935702-18-4
	SOL	71-43-2 Benzene
	CON	2 hours, reflux
RX(3)	RCT	G 935702-18-4
	RGT	J 7803-57-8 N ₂ H ₄ -H ₂ O
	PRO	I 935702-19-5
	SOL	64-17-5 EtOH
	CON	10 hours, reflux
RX(6)	RCT	I 935702-19-5, Q 104-88-1
	PRO	R 935702-22-0
	CAT	64-19-7 AcOH
	SOL	64-17-5 EtOH
	CON	reflux
RX(14)	RCT	R 935702-22-0, B 79-04-9
	RGT	AD 121-44-8 Et ₃ N
	PRO	AF 935702-30-0
	SOL	71-43-2 Benzene
	CON	SUBSTAGE(1) 50 deg C
		SUBSTAGE(2) room temperature
		SUBSTAGE(3) reflux

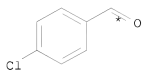
RX(92) OF 118 COMPOSED OF RX(2), RX(3), RX(6), RX(22)
 RX(92) C + F + Q + AL ==> AP



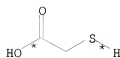
C



F



Q



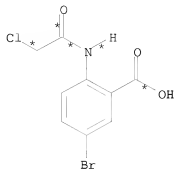
AL

4
 STEPS
 →

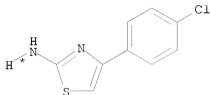
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2)	RCT	C 155104-20-4, F 2103-99-3
	RGT	H 584-08-7 K2CO3
	PRO	G 935702-18-4
	SOL	71-43-2 Benzene
	CON	2 hours, reflux
RX(3)	RCT	G 935702-18-4
	RGT	J 7803-57-8 N2H4-H2O
	PRO	I 935702-19-5
	SOL	64-17-5 EtOH
	CON	10 hours, reflux
RX(6)	RCT	I 935702-19-5, Q 104-88-1
	PRO	R 935702-22-0
	CAT	64-19-7 AcOH
	SOL	64-17-5 EtOH
	CON	reflux
RX(22)	RCT	R 935702-22-0, AL 68-11-1
	PRO	AP 935702-38-8
	CAT	7646-85-7 ZnCl2
	SOL	71-43-2 Benzene
	CON	SUBSTAGE(1) room temperature
		SUBSTAGE(2) reflux

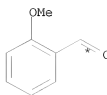
RX(93) OF 118 COMPOSED OF RX(2), RX(3), RX(7), RX(15)
 RX(93) C + F + S + B ==> AG



C



F



S



B

4
 STEPS
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

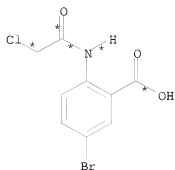
RX(2) RCT C 155104-20-4, F 2103-99-3
 RGT H 584-08-7 K₂CO₃
 PRO G 935702-18-4
 SOL 71-43-2 Benzene
 CON 2 hours, reflux

RX(3) RCT G 935702-18-4
 RGT J 7803-57-8 N₂H₄-H₂O
 PRO I 935702-19-5
 SOL 64-17-5 EtOH
 CON 10 hours, reflux

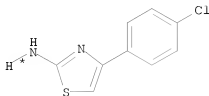
RX(7) RCT I 935702-19-5, S 135-02-4
 PRO T 935702-23-1
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON reflux

RX(15) RCT T 935702-23-1, B 79-04-9
 RGT AD 121-44-8 Et₃N
 PRO AG 935702-31-1
 SOL 71-43-2 Benzene
 CON SUBSTAGE(1) 50 deg C
 SUBSTAGE(2) room temperature
 SUBSTAGE(3) reflux

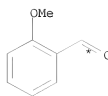
RX(94) OF 118 COMPOSED OF RX(2), RX(3), RX(7), RX(23)
 RX(94) C + F + S + AL ==> AQ



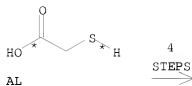
C



F



S



AL

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

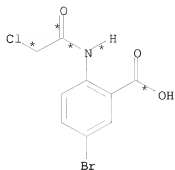
RX(2) RCT C 155104-20-4, F 2103-99-3
 RGT H 584-08-7 K2CO3
 PRO G 935702-18-4
 SOL 71-43-2 Benzene
 CON 2 hours, reflux

RX(3) RCT G 935702-18-4
 RGT J 7803-57-8 N2H4-H2O
 PRO I 935702-19-5
 SOL 64-17-5 EtOH
 CON 10 hours, reflux

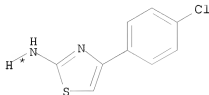
RX(7) RCT I 935702-19-5, S 135-02-4
 PRO T 935702-23-1
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON reflux

RX(23) RCT T 935702-23-1, AL 68-11-1
 PRO AQ 935702-39-9
 CAT 7646-85-7 ZnCl2
 SOL 71-43-2 Benzene
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) reflux

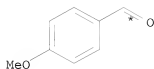
RX(95) OF 118 COMPOSED OF RX(2), RX(3), RX(8), RX(16)
 RX(95) C + F + U + B ==> AH



C



F



U



B



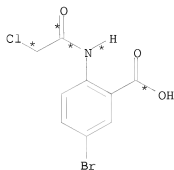
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2)	RCT	C 155104-20-4, F 2103-99-3
	RGT	H 584-08-7 K2CO3
	PRO	G 935702-18-4
	SOL	71-43-2 Benzene
	CON	2 hours, reflux
RX(3)	RCT	G 935702-18-4
	RGT	J 7803-57-8 N2H4-H2O
	PRO	I 935702-19-5
	SOL	64-17-5 EtOH
	CON	10 hours, reflux
RX(8)	RCT	I 935702-19-5, U 123-11-5
	PRO	V 935702-24-2
	CAT	64-19-7 AcOH
	SOL	64-17-5 EtOH
	CON	reflux
RX(16)	RCT	V 935702-24-2, B 79-04-9
	RGT	AD 121-44-8 Et3N
	PRO	AH 935702-32-2
	SOL	71-43-2 Benzene
	CON	SUBSTAGE(1) 50 deg C
		SUBSTAGE(2) room temperature

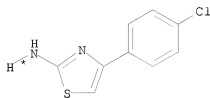
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SUBSTAGE(3) reflux

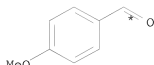
RX(96) OF 118 COMPOSED OF RX(2), RX(3), RX(8), RX(24)
 RX(96) C + F + U + AL ==> AR



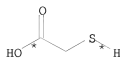
C



F



U



AL

4
 STEPS
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 155104-20-4, F 2103-99-3
 RGT H 584-08-7 K2CO3
 PRO G 935702-18-4
 SOL 71-43-2 Benzene
 CON 2 hours, reflux

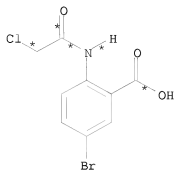
RX(3) RCT G 935702-18-4
 RGT J 7803-57-8 N2H4-H2O
 PRO I 935702-19-5
 SOL 64-17-5 EtOH
 CON 10 hours, reflux

RX(8) RCT I 935702-19-5, U 123-11-5
 PRO V 935702-24-2
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON reflux

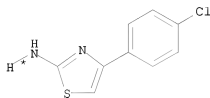
RX(24) RCT V 935702-24-2, AL 68-11-1
 PRO AR 935702-40-2
 CAT 7646-85-7 ZnCl2
 SOL 71-43-2 Benzene

CON SUBSTAGE(1) room temperature
SUBSTAGE(2) reflux

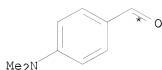
RX(97) OF 118 COMPOSED OF RX(2), RX(3), RX(9), RX(17)
RX(97) C + F + W + B ==> AI



C



F



W



B

4
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 155104-20-4, F 2103-99-3
RGT H 584-08-7 K₂CO₃
PRO G 935702-18-4
SOL 71-43-2 Benzene
CON 2 hours, reflux

RX(3) RCT G 935702-18-4
RGT J 7803-57-8 N₂H₄-H₂O
PRO I 935702-19-5
SOL 64-17-5 EtOH
CON 10 hours, reflux

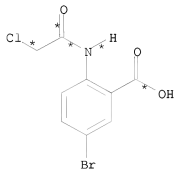
RX(9) RCT I 935702-19-5, W 100-10-7
PRO X 935702-25-3
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON reflux

RX(17) RCT X 935702-25-3, B 79-04-9
RGT AD 121-44-8 Et₃N
PRO AI 935702-33-3

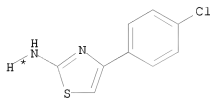
10/ 562,112

SOL 71-43-2 Benzene
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) room temperature
SUBSTAGE(3) reflux

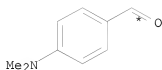
RX(98) OF 118 COMPOSED OF RX(2), RX(3), RX(9), RX(25)
RX(98) C + F + W + AL ==> AS



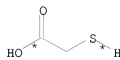
C



F



W



AL

4
STEPS
➔

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 155104-20-4, F 2103-99-3
RGT H 584-08-7 K2CO3
PRO G 935702-18-4
SOL 71-43-2 Benzene
CON 2 hours, reflux

RX(3) RCT G 935702-18-4
RGT J 7803-57-8 N2H4-H2O
PRO I 935702-19-5
SOL 64-17-5 EtOH
CON 10 hours, reflux

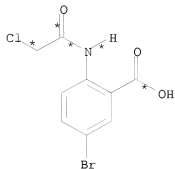
RX(9) RCT I 935702-19-5, W 100-10-7
PRO X 935702-25-3
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON reflux

RX(25) RCT X 935702-25-3, AL 68-11-1

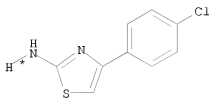
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PRO AS 935702-41-3
CAT 7646-85-7 ZnCl2
SOL 71-43-2 Benzene
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) reflux

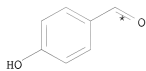
RX(99) OF 118 COMPOSED OF RX(2), RX(3), RX(10), RX(18)
RX(99) C + F + Y + B ==> AJ



C



F



Y



B

4
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 155104-20-4, F 2103-99-3
RGT H 584-08-7 K2CO3
PRO G 935702-18-4
SOL 71-43-2 Benzene
CON 2 hours, reflux

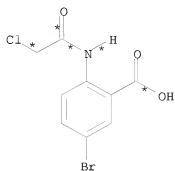
RX(3) RCT G 935702-18-4
RGT J 7803-57-8 N2H4-H2O
PRO I 935702-19-5
SOL 64-17-5 EtOH
CON 10 hours, reflux

RX(10) RCT I 935702-19-5, Y 123-08-0
PRO Z 935702-26-4
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH
CON reflux

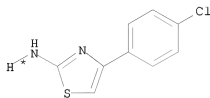
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RX(18) RCT Z 935702-26-4, B 79-04-9
RGT AD 121-44-8 Et3N
PRO AJ 935702-34-4
SOL 71-43-2 Benzene
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) room temperature
SUBSTAGE(3) reflux

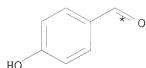
RX(100) OF 118 COMPOSED OF RX(2), RX(3), RX(10), RX(26)
RX(100) C + F + Y + AL ==> AT



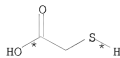
C



F



Y



AL

4
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 155104-20-4, F 2103-99-3
RGT H 584-08-7 K2CO3
PRO G 935702-18-4
SOL 71-43-2 Benzene
CON 2 hours, reflux

RX(3) RCT G 935702-18-4
RGT J 7803-57-8 N2H4-H2O
PRO I 935702-19-5
SOL 64-17-5 EtOH
CON 10 hours, reflux

RX(10) RCT I 935702-19-5, Y 123-08-0
PRO Z 935702-26-4
CAT 64-19-7 AcOH
SOL 64-17-5 EtOH

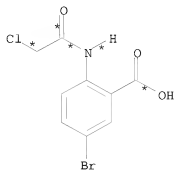
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CON reflux

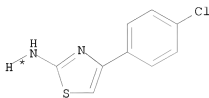
RX(26) RCT Z 935702-26-4, AL 68-11-1
PRO AT 935702-42-4
CAT 7646-85-7 ZnCl2
SOL 71-43-2 Benzene
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) reflux

RX(101) OF 118 COMPOSED OF RX(2), RX(3), RX(11), RX(19)

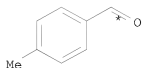
RX(101) C + F + AA + B ==> AK



C



F



AA



B

4
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 155104-20-4, F 2103-99-3
RGT H 584-08-7 K2CO3
PRO G 935702-18-4
SOL 71-43-2 Benzene
CON 2 hours, reflux

RX(3) RCT G 935702-18-4
RGT J 7803-57-8 N2H4-H2O
PRO I 935702-19-5
SOL 64-17-5 EtOH
CON 10 hours, reflux

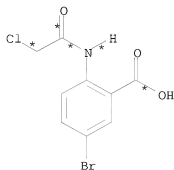
RX(11) RCT I 935702-19-5, AA 104-87-0
PRO AB 935702-27-5
CAT 64-19-7 AcOH

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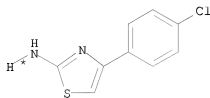
SOL 64-17-5 EtOH
CON reflux

RX(19) RCT AB 935702-27-5, B 79-04-9
RGT AD 121-44-8 Et3N
PRO AK 935702-35-5
SOL 71-43-2 Benzene
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) room temperature
SUBSTAGE(3) reflux

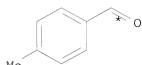
RX(102) OF 118 COMPOSED OF RX(2), RX(3), RX(11), RX(27)
RX(102) C + F + AA + AL ==> AU



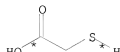
C



F



AA



AL

4
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT C 155104-20-4, F 2103-99-3
RGT H 584-08-7 K2CO3
PRO G 935702-18-4
SOL 71-43-2 Benzene
CON 2 hours, reflux

RX(3) RCT G 935702-18-4
RGT J 7803-57-8 N2H4-H2O
PRO I 935702-19-5
SOL 64-17-5 EtOH
CON 10 hours, reflux

RX(11) RCT I 935702-19-5, AA 104-87-0

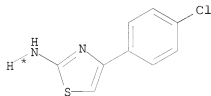
PRO AB 935702-27-5
 CAT 64-19-7 AcOH
 SOL 64-17-5 EtOH
 CON reflux

RX(27) RCT AB 935702-27-5, AL 68-11-1
 PRO AU 935702-43-5
 CAT 7646-85-7 ZnCl2
 SOL 71-43-2 Benzene
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) reflux

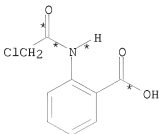
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 23 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 146:462201 CASREACT
 TITLE: Synthesis of N-3[4-(4-chlorophenyl
 thiazole-2-yl)-(2-(amino)methyl)-quinazoline-4(3H)-one
 and their derivatives for antitubercular activity
 AUTHOR(S): Pattan, Shashikant R.; Reddy, V. V. Krishna; Manvi, F.
 V.; Desai, B. G.; Bhat, A. R.
 CORPORATE SOURCE: Department of Medicinal Chemistry, K L E S's College
 of Pharmacy, Belgaum, 590 010, Belg.
 SOURCE: Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (2006),
 45B(7), 1778-1781
 CODEN: IJSBDB; ISSN: 0376-4699
 PUBLISHER: National Institute of Science Communication and
 Information Resources
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A new series of N-3[4-(4-chlorophenylthiazole-2-yl)-2-
 aminomethyl]quinazoline-4(3H)-one and their derivs. are synthesized. The
 structures of the title compds. are confirmed on the basis of IR and ¹H
 NMR. The compds. are screened for their antitubercular activity, using
 H37Rv strain on L J medium. All the compds. have showed moderate to
 promising antitubercular activity.

RX(3) OF 56 ...C + H ==> K...



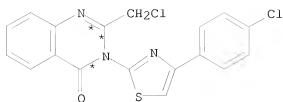
C



H

(3) →

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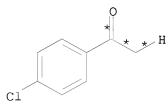


K
YIELD 58%

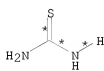
RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

RX(14) OF 56 COMPOSED OF RX(1), RX(3)

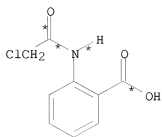
RX(14) A + B + H ==> K



A

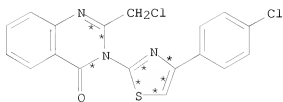


B



H

2
STEPS
→



K
YIELD 58%

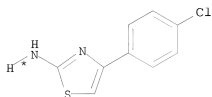
RX(1) RCT A 99-91-2, B 62-56-6

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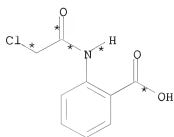
RGT D 7726-95-6 Br2
 PRO C 2103-99-3
 SOL 64-17-5 EtOH
 CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

RX(16) OF 56 COMPOSED OF RX(3), RX(4)
 RX(16) C + H + M ==> N



C



H



D1-NH2

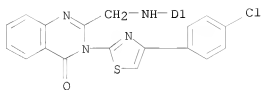
D1-Cl

M

2
 STEPS
 →



D1-Cl



N

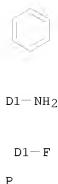
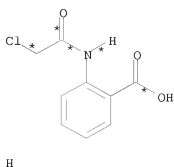
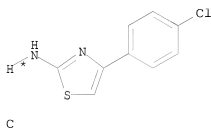
RX(3) RCT C 2103-99-3, H 14422-49-2

10/ 562,112

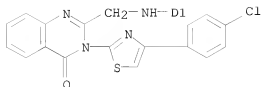
RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

RX(4) RCT M 27134-26-5, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO N 934817-07-9
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(17) OF 56 COMPOSED OF RX(3), RX(5)
 RX(17) C + H + P ==> Q



2
 STEPS
 →



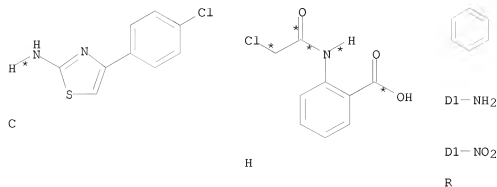
RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3

10/ 562,112

PRO K 870539-40-5
SOL 64-17-5 EtOH
CON 20 hours, reflux

RX(5) RCT P 87686-42-8, K 870539-40-5
RGT I 110-86-1 Pyridine
PRO Q 934817-08-0
SOL 108-24-7 Ac2O
CON 4 hours, reflux

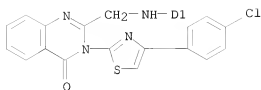
RX(18) OF 56 COMPOSED OF RX(3), RX(6)
RX(18) C + H + R ==> S



2
STEPS
→



D1-NO₂



S

RX(3) RCT C 2103-99-3, H 14422-49-2
RGT L 584-08-7 K₂CO₃
PRO K 870539-40-5

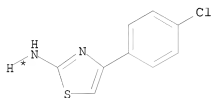
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SOL 64-17-5 EtOH
CON 20 hours, reflux

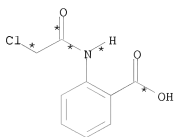
RX(6) RCT R 29757-24-2, K 870539-40-5
RGT I 110-86-1 Pyridine
PRO S 934817-09-1
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(19) OF 56 COMPOSED OF RX(3), RX(7)

RX(19) C + H + T ==> U



C



H



D1-NH₂

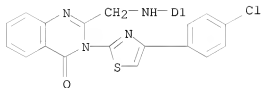
D1-Me

T

2
STEPS
=>



D1-Me



U

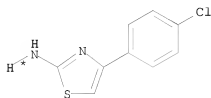
RX(3) RCT C 2103-99-3, H 14422-49-2
RGT L 584-08-7 K2CO3
PRO K 870539-40-5
SOL 64-17-5 EtOH

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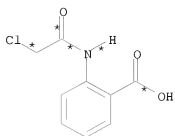
CON 20 hours, reflux

RX(7) RCT T 26915-12-8, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO U 934817-10-4
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(20) OF 56 COMPOSED OF RX(3), RX(8)
 RX(20) C + H + V ==> W



C



H



D1-NH2

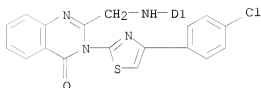
D1-O-Me

V

2
 STEPS
 →



D1-O-Me



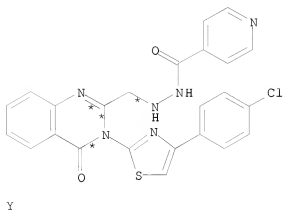
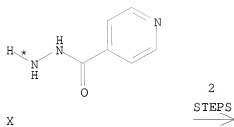
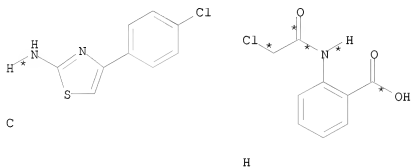
W

RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

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RX(8) RCT V 29191-52-4, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO W 934817-11-5
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(21) OF 56 COMPOSED OF RX(3), RX(9)
 RX(21) C + H + X ==> Y



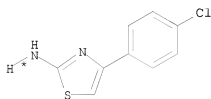
RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3
 PRO K 870539-40-5

10/ 562,112

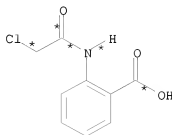
SOL 64-17-5 EtOH
CON 20 hours, reflux

RX(9) RCT X 54-85-3, K 870539-40-5
RGT I 110-86-1 Pyridine
PRO Y 934767-99-4
SOL 108-24-7 Ac2O
CON 4 hours, reflux

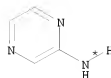
RX(22) OF 56 COMPOSED OF RX(3), RX(10)
RX(22) C + H + Z ==> AA



C

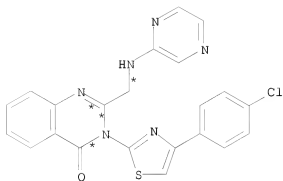


H



Z

2
STEPS
→



AA

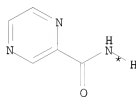
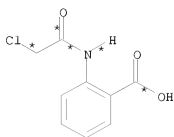
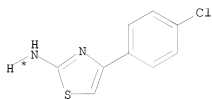
RX(3) RCT C 2103-99-3, H 14422-49-2
RGT L 584-08-7 K2CO3
PRO K 870539-40-5
SOL 64-17-5 EtOH
CON 20 hours, reflux

RX(10) RCT Z 5049-61-6, K 870539-40-5
RGT I 110-86-1 Pyridine

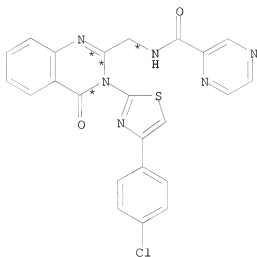
10/ 562,112

PRO AA 870539-37-0
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(23) OF 56 COMPOSED OF RX(3), RX(11)
RX(23) C + H + AB ==> AC



2
STEPS
→



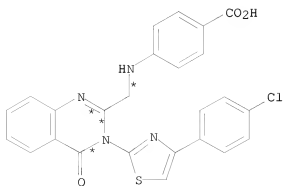
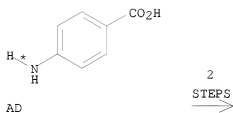
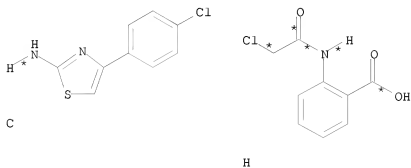
RX(3) RCT C 2103-99-3, H 14422-49-2
RGT L 584-08-7 K2CO3

10/ 562,112

PRO K 870539-40-5
SOL 64-17-5 EtOH
CON 20 hours, reflux

RX(11) RCT AB 98-96-4, K 870539-40-5
RGT I 110-86-1 Pyridine
PRO AC 870539-38-1
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(24) OF 56 COMPOSED OF RX(3), RX(12)
RX(24) C + H + AD ==> AE



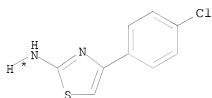
AE

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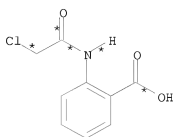
RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

RX(12) RCT AD 150-13-0, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO AE 934768-00-0
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

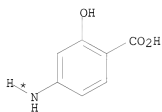
RX(25) OF 56 COMPOSED OF RX(3), RX(13)
 RX(25) C + H + AF ==> AG



C

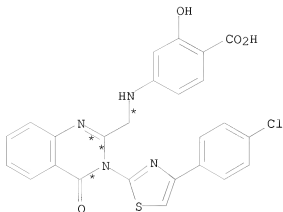


H



AF

2
 STEPS
 →



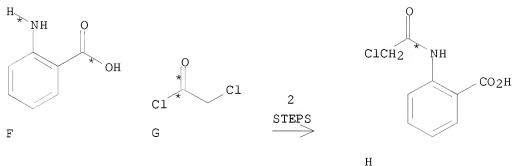
AG

RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

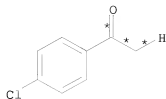
RX(13) RCT AF 65-49-6, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO AG 870539-39-2
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(26) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3)
 AND REACTION SEQUENCE RX(1), RX(3)

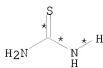
...F + G ==> H...
 ...A + B + H ==> K



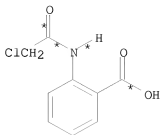
START NEXT REACTION SEQUENCE



A

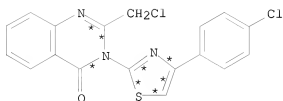


B



H

2
STEPS
→



K

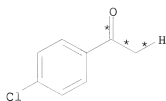
YIELD 58%

RX(2) RCT F 118-92-3, G 79-04-9
RGT I 110-86-1 Pyridine
PRO H 14422-49-2
SOL 71-43-2 Benzene
CON 4 hours, reflux

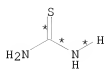
RX(1) RCT A 99-91-2, B 62-56-6
RGT D 7726-95-6 Br2
PRO C 2103-99-3
SOL 64-17-5 EtOH
CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2
RGT L 584-08-7 K2CO3
PRO K 870539-40-5
SOL 64-17-5 EtOH
CON 20 hours, reflux

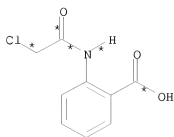
RX(27) OF 56 COMPOSED OF RX(1), RX(3), RX(4)
RX(27) A + B + H + M ==> N



A



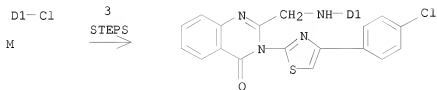
B



H

D1-NH₂

D1-Cl

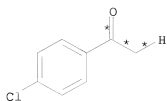


N

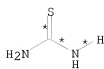
RX(1)	RCT	A 99-91-2, B 62-56-6
	RGT	D 7726-95-6 Br ₂
	PRO	C 2103-99-3
	SOL	64-17-5 EtOH
	CON	overnight, reflux
RX(3)	RCT	C 2103-99-3, H 14422-49-2
	RGT	L 584-08-7 K ₂ CO ₃
	PRO	K 870539-40-5
	SOL	64-17-5 EtOH
	CON	20 hours, reflux
RX(4)	RCT	M 27134-26-5, K 870539-40-5
	RGT	I 110-86-1 Pyridine
	PRO	N 934817-07-9
	SOL	108-24-7 Ac ₂ O
	CON	4 hours, reflux

RX(28) OF 56 COMPOSED OF RX(1), RX(3), RX(5)

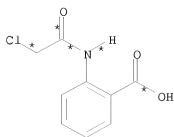
RX(28) A + B + H + P ==> Q



A



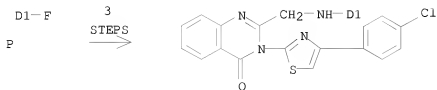
B



H

D1-NH₂

D1-F

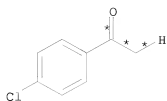


Q

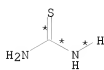
RX(1)	RCT	A 99-91-2, B 62-56-6
	RGT	D 7726-95-6 Br ₂
	PRO	C 2103-99-3
	SOL	64-17-5 EtOH
	CON	overnight, reflux
RX(3)	RCT	C 2103-99-3, H 14422-49-2
	RGT	L 584-08-7 K ₂ CO ₃
	PRO	K 870539-40-5
	SOL	64-17-5 EtOH
	CON	20 hours, reflux
RX(5)	RCT	P 87686-42-8, K 870539-40-5
	RGT	I 110-86-1 Pyridine
	PRO	Q 934817-08-0
	SOL	108-24-7 Ac ₂ O
	CON	4 hours, reflux

RX(29) OF 56 COMPOSED OF RX(1), RX(3), RX(6)

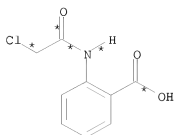
RX(29) A + B + H + R ==> S



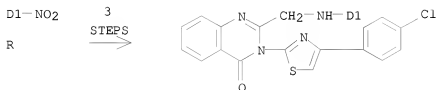
A



B



H

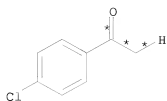
D1-NH₂D1-NO₂

S

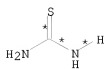
RX(1)	RCT	A 99-91-2, B 62-56-6
	RGT	D 7726-95-6 Br ₂
	PRO	C 2103-99-3
	SOL	64-17-5 EtOH
	CON	overnight, reflux
RX(3)	RCT	C 2103-99-3, H 14422-49-2
	RGT	L 584-08-7 K ₂ CO ₃
	PRO	K 870539-40-5
	SOL	64-17-5 EtOH
	CON	20 hours, reflux
RX(6)	RCT	R 29757-24-2, K 870539-40-5
	RGT	I 110-86-1 Pyridine
	PRO	S 934817-09-1
	SOL	108-24-7 Ac ₂ O
	CON	4 hours, reflux

RX(30) OF 56 COMPOSED OF RX(1), RX(3), RX(7)

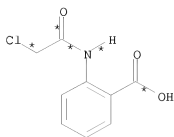
RX(30) A + B + H + T ==> U



A



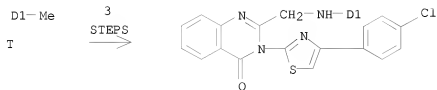
B



H

D1-NH₂

D1-Me

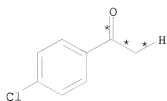


U

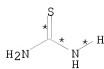
RX(1)	RCT	A 99-91-2, B 62-56-6
	RGT	D 7726-95-6 Br ₂
	PRO	C 2103-99-3
	SOL	64-17-5 EtOH
	CON	overnight, reflux
RX(3)	RCT	C 2103-99-3, H 14422-49-2
	RGT	L 584-08-7 K ₂ CO ₃
	PRO	K 870539-40-5
	SOL	64-17-5 EtOH
	CON	20 hours, reflux
RX(7)	RCT	T 26915-12-8, K 870539-40-5
	RGT	I 110-86-1 Pyridine
	PRO	U 934817-10-4
	SOL	108-24-7 Ac ₂ O
	CON	4 hours, reflux

RX(31) OF 56 COMPOSED OF RX(1), RX(3), RX(8)

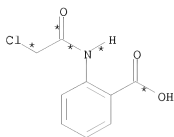
RX(31) A + B + H + V ==> W



A



B



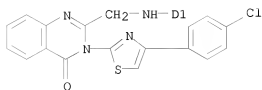
H

D1-NH₂

D1-O-Me

D1-O-Me

V

 3
 STEPS
 →


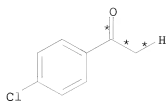
W

RX(1) RCT A 99-91-2, B 62-56-6
 RGT D 7726-95-6 Br₂
 PRO C 2103-99-3
 SOL 64-17-5 EtOH
 CON overnight, reflux

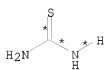
 RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K₂CO₃
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

 RX(8) RCT V 29191-52-4, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO W 934817-11-5
 SOL 108-24-7 Ac₂O
 CON 4 hours, reflux

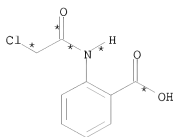
RX(32) OF 56 COMPOSED OF RX(1), RX(3), RX(9)
 RX(32) A + B + H + X ==> Y



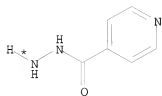
A



B

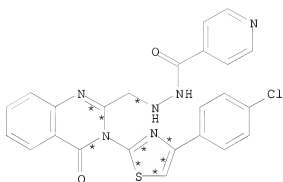


H



X

3
STEPS
→



Y

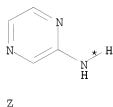
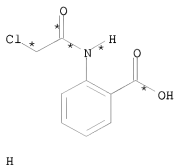
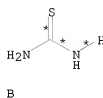
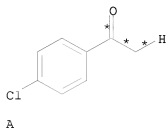
RX(1) RCT A 99-91-2, B 62-56-6
RGT D 7726-95-6 Br2
PRO C 2103-99-3
SOL 64-17-5 EtOH
CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2
RGT L 584-08-7 K2CO3
PRO K 870539-40-5
SOL 64-17-5 EtOH
CON 20 hours, reflux

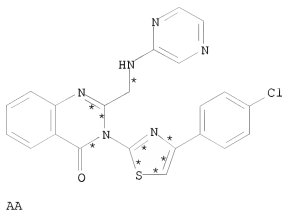
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RX(9) RCT X 54-85-3, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO Y 934767-99-4
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(33) OF 56 COMPOSED OF RX(1), RX(3), RX(10)
 RX(33) A + B + H + Z ==> AA



3
 STEPS
 →



RX(1) RCT A 99-91-2, B 62-56-6
 RGT D 7726-95-6 Br2
 PRO C 2103-99-3
 SOL 64-17-5 EtOH
 CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

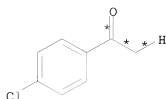
RX(10) RCT Z 5049-61-6, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO AA 870539-37-0
 SOL 108-24-7 Ac2O

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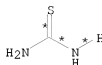
CON 4 hours, reflux

RX(34) OF 56 COMPOSED OF RX(1), RX(3), RX(11)

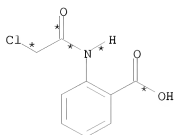
RX(34) A + B + H + AB ==> AC



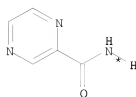
A



B

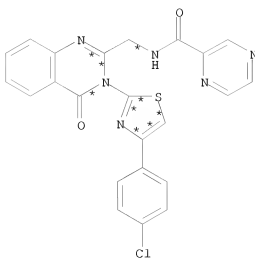


H



AB

3
STEPS
→



AC

RX(1) RCT A 99-91-2, B 62-56-6
RGT D 7726-95-6 Br2
PRO C 2103-99-3
SOL 64-17-5 EtOH
CON overnight, reflux

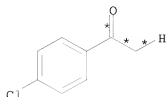
RX(3) RCT C 2103-99-3, H 14422-49-2
RGT L 584-08-7 K2CO3
PRO K 870539-40-5
SOL 64-17-5 EtOH
CON 20 hours, reflux

RX(11) RCT AB 98-96-4, K 870539-40-5
RGT I 110-86-1 Pyridine
PRO AC 870539-38-1

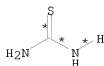
10/ 562,112

SOL 108-24-7 Ac2O
CON 4 hours, reflux

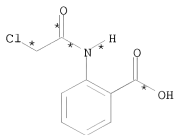
RX(35) OF 56 COMPOSED OF RX(1), RX(3), RX(12)
RX(35) A + B + H + AD ==> AE



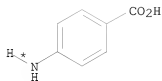
A



B

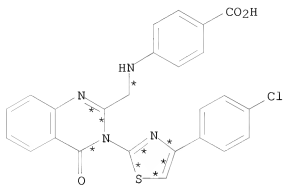


H



AD

3
STEPS
→



AE

RX(1) RCT A 99-91-2, B 62-56-6
RGT D 7726-95-6 Br2
PRO C 2103-99-3
SOL 64-17-5 EtOH
CON overnight, reflux

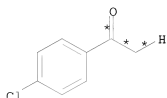
RX(3) RCT C 2103-99-3, H 14422-49-2

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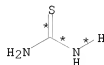
RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

RX(12) RCT AD 150-13-0, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO AE 934768-00-0
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

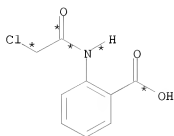
RX(36) OF 56 COMPOSED OF RX(1), RX(3), RX(13)
 RX(36) A + B + H + AF ==> AG



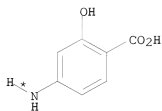
A



B

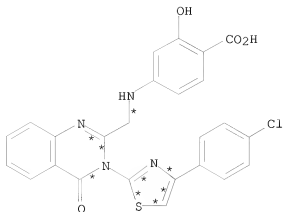


H



AF

3
 STEPS
 →



AG

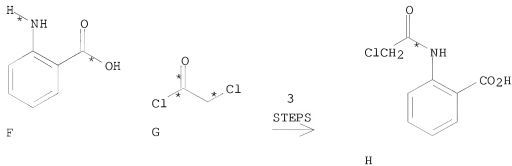
RX(1) RCT A 99-91-2, B 62-56-6
 RGT D 7726-95-6 Br2
 PRO C 2103-99-3
 SOL 64-17-5 EtOH
 CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

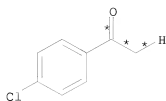
RX(13) RCT AF 65-49-6, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO AG 870539-39-2
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(47) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(4)
 AND REACTION SEQUENCE RX(1), RX(3), RX(4)

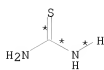
...F + G ==> H...
 ...A + B + H + M ==> N



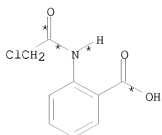
START NEXT REACTION SEQUENCE



A



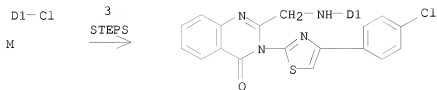
B



H

D1-NH₂

D1-Cl



N

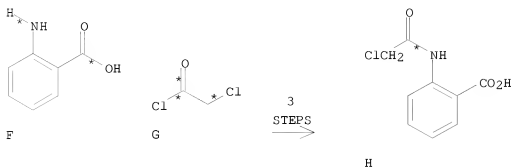
RX(2)	RCT	F 118-92-3, G 79-04-9
	RGT	I 110-86-1 Pyridine
	PRO	H 14422-49-2
	SOL	71-43-2 Benzene
	CON	4 hours, reflux
RX(1)	RCT	A 99-91-2, B 62-56-6
	RGT	D 7726-95-6 Br ₂
	PRO	C 2103-99-3
	SOL	64-17-5 EtOH
	CON	overnight, reflux
RX(3)	RCT	C 2103-99-3, H 14422-49-2
	RGT	L 584-08-7 K ₂ CO ₃
	PRO	K 870539-40-5
	SOL	64-17-5 EtOH
	CON	20 hours, reflux
RX(4)	RCT	M 27134-26-5, K 870539-40-5
	RGT	I 110-86-1 Pyridine
	PRO	N 934817-07-9
	SOL	108-24-7 Ac ₂ O

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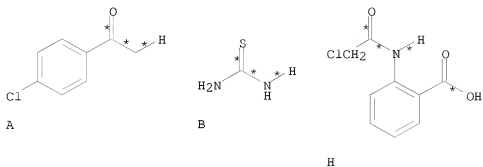
CON 4 hours, reflux

RX(48) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(5)
AND REACTION SEQUENCE RX(1), RX(3), RX(5)

...F + G ==> H...
...A + B + H + P ==> Q



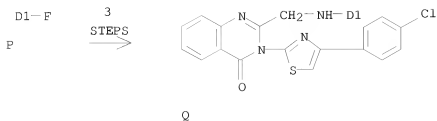
START NEXT REACTION SEQUENCE



D1-NH₂



D1-F



RX(2) RCT F 118-92-3, G 79-04-9
 RGT I 110-86-1 Pyridine
 PRO H 14422-49-2
 SOL 71-43-2 Benzene
 CON 4 hours, reflux

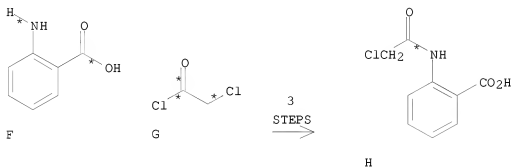
 RX(1) RCT A 99-91-2, B 62-56-6
 RGT D 7726-95-6 Br2
 PRO C 2103-99-3
 SOL 64-17-5 EtOH
 CON overnight, reflux

 RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

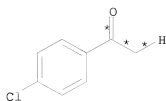
 RX(5) RCT P 87686-42-8, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO Q 934817-08-0
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(49) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(6)
 AND REACTION SEQUENCE RX(1), RX(3), RX(6)

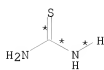
...F + G ==> H...
 ...A + B + H + R ==> S



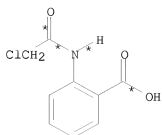
START NEXT REACTION SEQUENCE



A



B

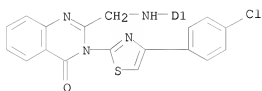


H

D1-NH₂D1-NO₂D1-NO₂

R

3
STEPS
→



S

RX(2)	RCT	F 118-92-3, G 79-04-9
	RGT	I 110-86-1 Pyridine
	PRO	H 14422-49-2
	SOL	71-43-2 Benzene
	CON	4 hours, reflux
RX(1)	RCT	A 99-91-2, B 62-56-6
	RGT	D 7726-95-6 Br ₂
	PRO	C 2103-99-3
	SOL	64-17-5 EtOH
	CON	overnight, reflux
RX(3)	RCT	C 2103-99-3, H 14422-49-2
	RGT	L 584-08-7 K ₂ CO ₃
	PRO	K 870539-40-5
	SOL	64-17-5 EtOH
	CON	20 hours, reflux
RX(6)	RCT	R 29757-24-2, K 870539-40-5
	RGT	I 110-86-1 Pyridine
	PRO	S 934817-09-1
	SOL	108-24-7 Ac ₂ O

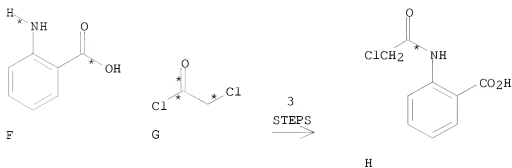
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CON 4 hours, reflux

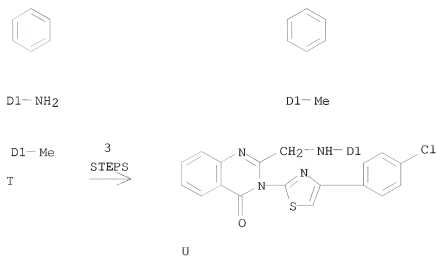
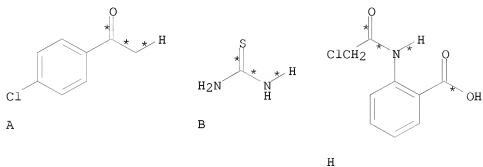
RX(50) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(7)
AND REACTION SEQUENCE RX(1), RX(3), RX(7)

...F + G ==> H...

...A + B + H + T ==> U



START NEXT REACTION SEQUENCE



RX(2) RCT F 118-92-3, G 79-04-9
 RGT I 110-86-1 Pyridine
 PRO H 14422-49-2
 SOL 71-43-2 Benzene
 CON 4 hours, reflux

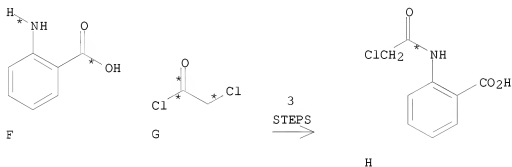
 RX(1) RCT A 99-91-2, B 62-56-6
 RGT D 7726-95-6 Br2
 PRO C 2103-99-3
 SOL 64-17-5 EtOH
 CON overnight, reflux

 RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

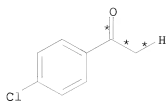
 RX(7) RCT T 26915-12-8, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO U 934817-10-4
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

RX(51) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(8)
 AND REACTION SEQUENCE RX(1), RX(3), RX(8)

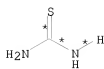
...F + G ==> H...
 ...A + B + H + V ==> W



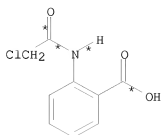
START NEXT REACTION SEQUENCE



A



B



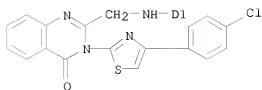
H

D1-NH₂

D1-O-Me

D1-O-Me

V

 3
 STEPS
 →


W

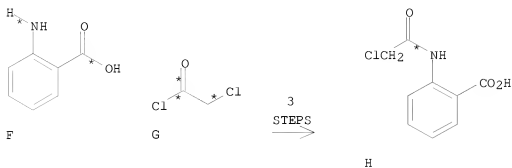
RX(2)	RCT	F 118-92-3, G 79-04-9
	RGT	I 110-86-1 Pyridine
	PRO	H 14422-49-2
	SOL	71-43-2 Benzene
	CON	4 hours, reflux
RX(1)	RCT	A 99-91-2, B 62-56-6
	RGT	D 7726-95-6 Br ₂
	PRO	C 2103-99-3
	SOL	64-17-5 EtOH
	CON	overnight, reflux
RX(3)	RCT	C 2103-99-3, H 14422-49-2
	RGT	L 584-08-7 K ₂ CO ₃
	PRO	K 870539-40-5
	SOL	64-17-5 EtOH
	CON	20 hours, reflux
RX(8)	RCT	V 29191-52-4, K 870539-40-5
	RGT	I 110-86-1 Pyridine
	PRO	W 934817-11-5
	SOL	108-24-7 Ac ₂ O

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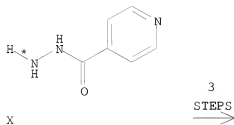
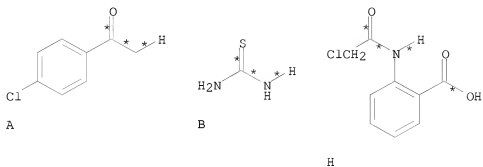
CON 4 hours, reflux

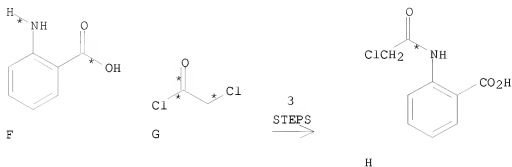
RX(52) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(9)
AND REACTION SEQUENCE RX(1), RX(3), RX(9)

...F + G ==> H...
...A + B + H + X ==> Y

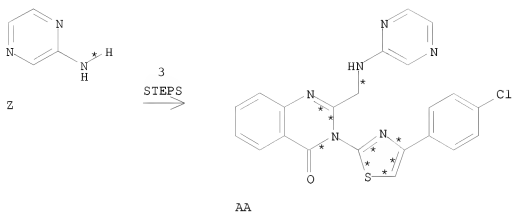
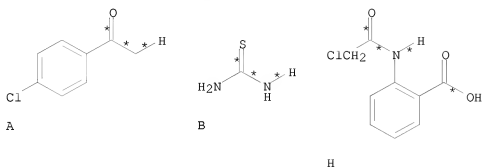


START NEXT REACTION SEQUENCE





START NEXT REACTION SEQUENCE



RX(2) RCT F 118-92-3, G 79-04-9
 RGT I 110-86-1 Pyridine
 PRO H 14422-49-2
 SOL 71-43-2 Benzene
 CON 4 hours, reflux

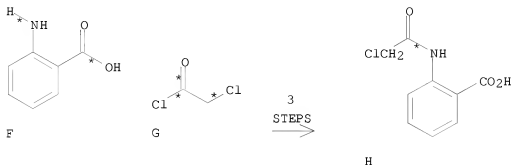
RX(1) RCT A 99-91-2, B 62-56-6
 RGT D 7726-95-6 Br2
 PRO C 2103-99-3
 SOL 64-17-5 EtOH
 CON overnight, reflux

RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

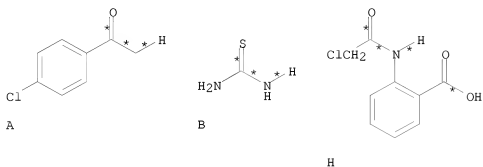
RX(10) RCT Z 5049-61-6, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO AA 870539-37-0
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

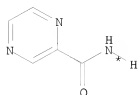
RX(54) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(11)
 AND REACTION SEQUENCE RX(1), RX(3), RX(11)

...F + G ==> H...
 ...A + B + H + AB ==> AC



START NEXT REACTION SEQUENCE





AB

3
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT F 118-92-3, G 79-04-9
RGT I 110-86-1 Pyridine
PRO H 14422-49-2
SOL 71-43-2 Benzene
CON 4 hours, reflux

RX(1) RCT A 99-91-2, B 62-56-6
RGT D 7726-95-6 Br2
PRO C 2103-99-3
SOL 64-17-5 EtOH
CON overnight, reflux

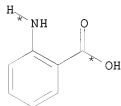
RX(3) RCT C 2103-99-3, H 14422-49-2
RGT L 584-08-7 K2CO3
PRO K 870539-40-5
SOL 64-17-5 EtOH
CON 20 hours, reflux

RX(11) RCT AB 98-96-4, K 870539-40-5
RGT I 110-86-1 Pyridine
PRO AC 870539-38-1
SOL 108-24-7 Ac2O
CON 4 hours, reflux

RX(55) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(12)
AND REACTION SEQUENCE RX(1), RX(3), RX(12)

...F + G ==> H...

...A + B + H + AD ==> AE

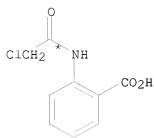


F



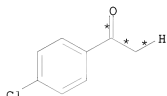
G

3
STEPS
→

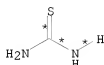


H

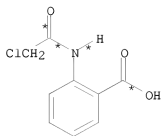
START NEXT REACTION SEQUENCE



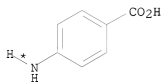
A



B

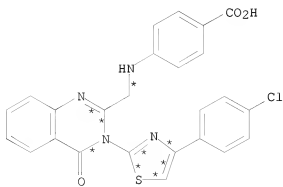


H



AD

3
STEPS
→



AE

RX(2) RCT F 118-92-3, G 79-04-9
 RGT I 110-86-1 Pyridine
 PRO H 14422-49-2
 SOL 71-43-2 Benzene
 CON 4 hours, reflux

RX(1) RCT A 99-91-2, B 62-56-6
 RGT D 7726-95-6 Br2
 PRO C 2103-99-3
 SOL 64-17-5 EtOH
 CON overnight, reflux

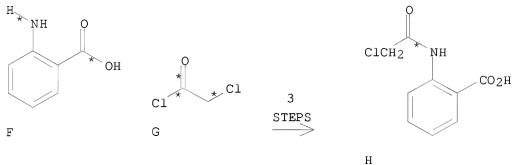
RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux

RX(12) RCT AD 150-13-0, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO AE 934768-00-0
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

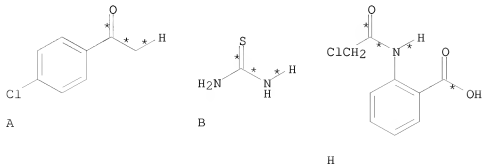
RX(56) OF 56 COMPOSED OF REACTION SEQUENCE RX(2), RX(3), RX(13)
 AND REACTION SEQUENCE RX(1), RX(3), RX(13)

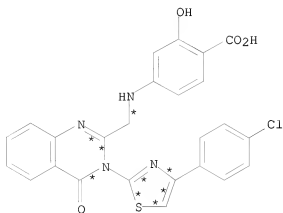
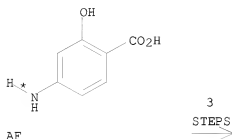
...F + G ==> H...

...A + B + H + AF ==> AG



START NEXT REACTION SEQUENCE





- RX(2) RCT F 118-92-3, G 79-04-9
 RGT I 110-86-1 Pyridine
 PRO H 14422-49-2
 SOL 71-43-2 Benzene
 CON 4 hours, reflux
- RX(1) RCT A 99-91-2, B 62-56-6
 RGT D 7726-95-6 Br2
 PRO C 2103-99-3
 SOL 64-17-5 EtOH
 CON overnight, reflux
- RX(3) RCT C 2103-99-3, H 14422-49-2
 RGT L 584-08-7 K2CO3
 PRO K 870539-40-5
 SOL 64-17-5 EtOH
 CON 20 hours, reflux
- RX(13) RCT AF 65-49-6, K 870539-40-5
 RGT I 110-86-1 Pyridine
 PRO AG 870539-39-2
 SOL 108-24-7 Ac2O
 CON 4 hours, reflux

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 24 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 146:421942 CASREACT

TITLE: Synthesis and behavior of 2-carboxyvinyl-6,8-dibromo-4H-3,1-benzoxazin-4-one towards nitrogen, carbon and sulphur nucleophiles

AUTHOR(S): El-Hashash, M. A.; Abdel-Rahman, T. M.; El-Badry, Y. A.

CORPORATE SOURCE: Faculty of Science, Ain Shams University, Cairo, Egypt

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2006), 45B(6), 1470-1477

CODEN: IJSBDB; ISSN: 0376-4699

PUBLISHER: National Institute of Science Communication and Information Resources

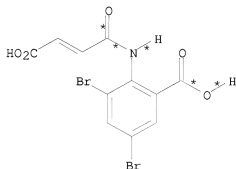
DOCUMENT TYPE: Journal

LANGUAGE: English

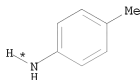
AB 3-(6,8-Dibromo-4-oxo-4H-3,1-benzoxazin-2-yl)-2-propenoic acid (I) is synthesized and allowed to react with some nitrogen nucleophiles namely, p-toluidine, hydroxylamine hydrochloride, ethanolamine, and glycine and affords 3-substituted quinazolinones, while with isobutylamine and benzylamine results benzamide derivs. Treatment of benzoxazinone I with o-phenylenediamine in different solvents under different conditions affords substituted benzamide and 3-substituted quinazolinone derivative

RX(33) OF 101 COMPOSED OF RX(2), RX(3)

RX(33) C + G ==> H

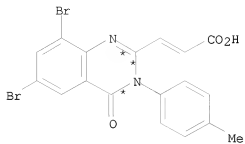


C



G

2
STEPS
→

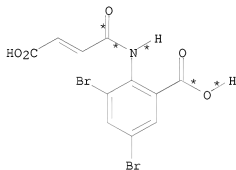


H
YIELD 48%

RX(2) RCT C 934242-55-4
RGT F 108-24-7 Ac2O
PRO E 838868-31-8
SOL 108-24-7 Ac2O
CON 1 hour, heated

RX(3) RCT E 838868-31-8, G 106-49-0
PRO H 934242-56-5
SOL 64-19-7 AcOH
CON 3 hours, reflux

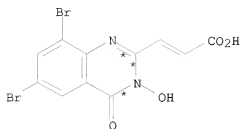
RX(34) OF 101 COMPOSED OF RX(2), RX(4)
RX(34) C ==> J



C

2
STEPS
→

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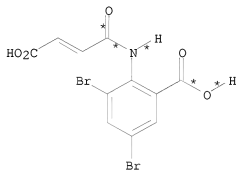


J
YIELD 73%

RX(2) RCT C 934242-55-4
RGT F 108-24-7 Ac2O
PRO E 838868-31-8
SOL 108-24-7 Ac2O
CON 1 hour, heated

RX(4) RCT E 838868-31-8
RGT K 5470-11-1 H2NOH-HCl
PRO J 934242-57-6
SOL 110-86-1 Pyridine
CON 3 hours, reflux

RX(35) OF 101 COMPOSED OF RX(2), RX(5)
RX(35) C + M ==> N



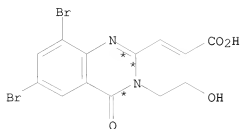
C



M

2
STEPS
→

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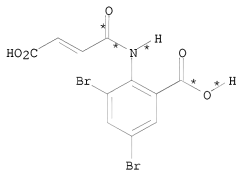


N
YIELD 58%

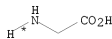
RX(2) RCT C 934242-55-4
RGT F 108-24-7 Ac2O
PRO E 838868-31-8
SOL 108-24-7 Ac2O
CON 1 hour, heated

RX(5) RCT E 838868-31-8, M 141-43-5
RGT O 127-09-3 AcONa
PRO N 934242-58-7
SOL 64-19-7 AcOH
CON 3 hours, reflux

RX(36) OF 101 COMPOSED OF RX(2), RX(6)
RX(36) C + P ==> Q



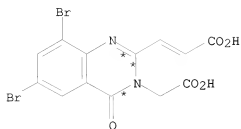
C



P

2
STEPS
→

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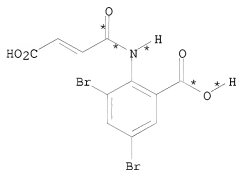


Q
YIELD 44%

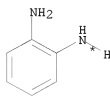
RX(2) RCT C 934242-55-4
RGT F 108-24-7 Ac2O
PRO E 838868-31-8
SOL 108-24-7 Ac2O
CON 1 hour, heated

RX(6) RCT E 838868-31-8, P 56-40-6
PRO Q 934242-59-8
SOL 110-86-1 Pyridine
CON 8 hours, reflux

RX(40) OF 101 COMPOSED OF RX(2), RX(15)
RX(40) C + AJ ==> AL



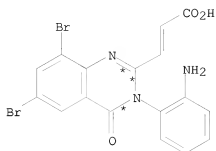
C



AJ

2
STEPS
➡

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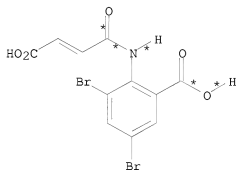


AL
YIELD 56%

RX(2) RCT C 934242-55-4
RGT F 108-24-7 Ac2O
PRO E 838868-31-8
SOL 108-24-7 Ac2O
CON 1 hour, heated

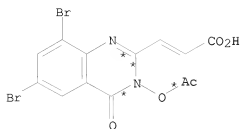
RX(15) RCT E 838868-31-8, AJ 95-54-5
RGT O 127-09-3 AcONa
PRO AL 934242-68-9
SOL 64-19-7 AcOH
CON 2 hours, reflux

RX(41) OF 101 COMPOSED OF RX(2), RX(16)
RX(41) C ==> AM



C

2
STEPS
→



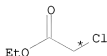
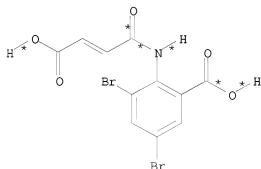
W
YIELD 80%

RX(2) RCT C 934242-55-4
RGT F 108-24-7 Ac2O
PRO E 838868-31-8
SOL 108-24-7 Ac2O
CON 1 hour, heated

RX(4) RCT E 838868-31-8
RGT K 5470-11-1 H2NOH-HCl
PRO J 934242-57-6
SOL 110-86-1 Pyridine
CON 3 hours, reflux

RX(9) RCT J 934242-57-6, F 108-24-7
PRO W 934242-62-3
SOL 108-24-7 Ac2O
CON 2 hours, reflux

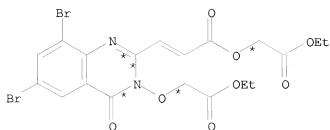
RX(82) OF 101 COMPOSED OF RX(2), RX(4), RX(10)
RX(82) C + 2 X ==> Y



C

2 X

3
STEPS
→



Y
YIELD 28%

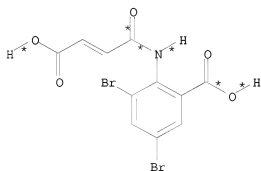
RX(2) RCT C 934242-55-4
RGT F 108-24-7 Ac2O
PRO E 838868-31-8
SOL 108-24-7 Ac2O
CON 1 hour, heated

RX(4) RCT E 838868-31-8
RGT K 5470-11-1 H2NOH-HCl
PRO J 934242-57-6
SOL 110-86-1 Pyridine
CON 3 hours, reflux

RX(10) RCT J 934242-57-6, X 105-39-5
RGT Z 584-08-7 K2CO3
PRO Y 934242-63-4
SOL 67-64-1 Me2CO
CON 24 hours, reflux

RX(83) OF 101 COMPOSED OF RX(2), RX(4), RX(11)

RX(83) C + 2 AB ==> AC



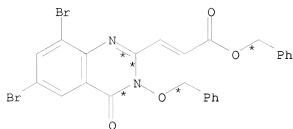
C



2 AB

3
STEPS
=>

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AC

YIELD 37%

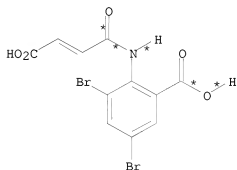
RX(2) RCT C 934242-55-4
 RGT F 108-24-7 Ac2O
 PRO E 838868-31-8
 SOL 108-24-7 Ac2O
 CON 1 hour, heated

RX(4) RCT E 838868-31-8
 RGT K 5470-11-1 H2NOH-HCl
 PRO J 934242-57-6
 SOL 110-86-1 Pyridine
 CON 3 hours, reflux

RX(11) RCT J 934242-57-6, AB 100-44-7
 RGT Z 584-08-7 K2CO3
 PRO AC 934242-64-5
 SOL 67-64-1 Me2CO
 CON 24 hours, reflux

RX(84) OF 101 COMPOSED OF RX(2), RX(5), RX(12)

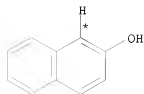
RX(84) C + M + AD ==> AE



C

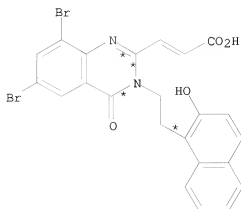


M



AD

3
 STEPS
 →



AE

YIELD 38%

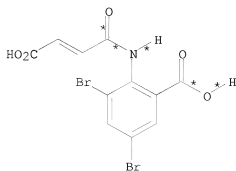
RX(2) RCT C 934242-55-4
 RGT F 108-24-7 Ac2O
 PRO E 838868-31-8
 SOL 108-24-7 Ac2O
 CON 1 hour, heated

RX(5) RCT E 838868-31-8, M 141-43-5
 RGT O 127-09-3 AcONa
 PRO N 934242-58-7
 SOL 64-19-7 AcOH
 CON 3 hours, reflux

RX(12) RCT N 934242-58-7, AD 135-19-3
 RGT AF 7732-18-5 Water
 PRO AE 934242-65-6
 CAT 7647-01-0 HCl
 SOL 64-17-5 EtOH
 CON 6 hours, heated

RX(85) OF 101 COMPOSED OF RX(2), RX(5), RX(13)

RX(85) C + M + AH ==> AI



C

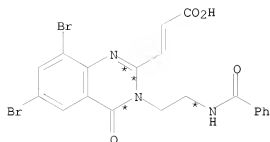


M



AH

3
STEPS
→



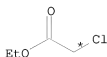
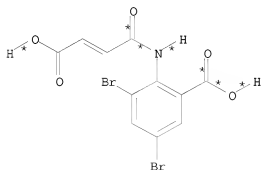
AI
YIELD 44%

RX(2) RCT C 934242-55-4
RGT F 108-24-7 Ac2O
PRO E 838868-31-8
SOL 108-24-7 Ac2O
CON 1 hour, heated

RX(5) RCT E 838868-31-8, M 141-43-5
RGT O 127-09-3 AcONa
PRO N 934242-58-7
SOL 64-19-7 AcOH
CON 3 hours, reflux

RX(13) RCT N 934242-58-7, AH 55-21-0
RGT AF 7732-18-5 Water
PRO AI 934242-66-7
CAT 7647-01-0 HCl
SOL 64-17-5 EtOH
CON 6 hours, heated

RX(86) OF 101 COMPOSED OF RX(2), RX(16), RX(17)
RX(86) C + 2 X ==> AO

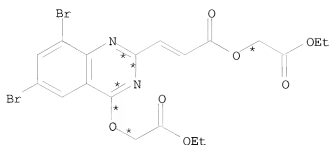


3
STEPS
→

C

2 X

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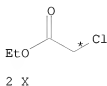
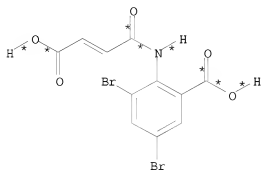
AO
YIELD 32%

RX(2) RCT C 934242-55-4
RGT F 108-24-7 Ac2O
PRO E 838868-31-8
SOL 108-24-7 Ac2O
CON 1 hour, heated

RX(16) RCT E 838868-31-8
RGT AN 75-12-7 Formamide
PRO AM 934242-69-0
SOL 75-12-7 Formamide
CON 2 hours, reflux

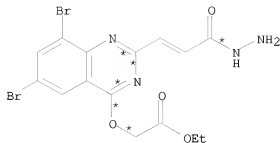
RX(17) RCT AM 934242-69-0, X 105-39-5
RGT Z 584-08-7 K2CO3
PRO AO 934242-70-3
SOL 67-64-1 Me2CO
CON 25 hours, reflux

RX(100) OF 101 COMPOSED OF RX(2), RX(16), RX(17), RX(18)
RX(100) C + 2 X ==> AP



4
STEPS
→

C



AP
YIELD 57%

RX(2) RCT C 934242-55-4
RGT F 108-24-7 Ac2O
PRO E 838868-31-8
SOL 108-24-7 Ac2O
CON 1 hour, heated

RX(16) RCT E 838868-31-8
RGT AN 75-12-7 Formamide
PRO AM 934242-69-0
SOL 75-12-7 Formamide
CON 2 hours, reflux

RX(17) RCT AM 934242-69-0, X 105-39-5
RGT Z 584-08-7 K2CO3
PRO AO 934242-70-3
SOL 67-64-1 Me2CO
CON 25 hours, reflux

RX(18) RCT AO 934242-70-3
RGT AQ 7803-57-8 N2H4-H2O
PRO AP 934242-71-4
SOL 64-17-5 EtOH
CON 6 hours, reflux
NTE regioselective

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 25 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 146:421939 CASREACT
TITLE: Diastereoselective synthesis of atropisomeric
3-(2-substituted aryl)quinazolin-4-ones and their
stereochemical properties

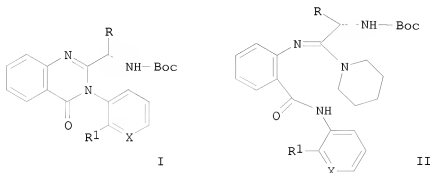
AUTHOR(S): Tokitoh, Takashi; Kobayashi, Toshitake; Nakada,
Eisuke; Inoue, Tohru; Yokoshima, Satoshi; Takahashi,
Hideyo; Natsugari, Hideaki

CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, The
University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo,
113-0033, Japan

SOURCE: Heterocycles (2006), 70, 93-99

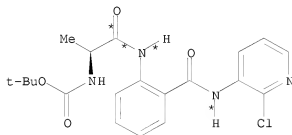
PUBLISHER:
DOCUMENT TYPE:
LANGUAGE:
GI

CODEN: HTCYAM; ISSN: 0385-5414
Japan Institute of Heterocyclic Chemistry
Journal
English



AB Atropisomeric [1-(3-aryl-4-oxo-3,4-dihydroquinazolin-2-yl)ethyl- and -phenethyl]carbamates I (X = N, R = Me, R1 = Cl; X = N, R = PhCH2, R1 = Cl; X = CH, R = PhCH2, R1 = CO2Me) were diastereoselectively synthesized by acid-catalyzed cyclization of appropriate {2-[(arylcabamoyl)phenylimino]-1-methyl- and -1-benzyl-2-piperidin-1-yl}carbamates II. Investigation of the stereochem. properties of I revealed that both atropisomers have high stereochem. stability and the (aR*, S*)- is stereochem. more stable than the isomeric (aS*, S*)-form.

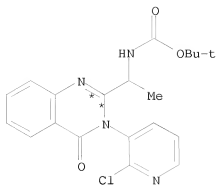
RX(1) OF 30 ...2 A ==> B + C



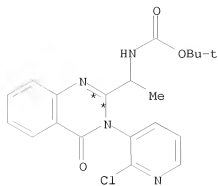
2 A



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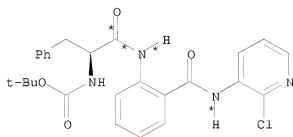
B
YIELD 38%



C
YIELD 42%

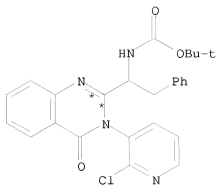
RX(1) RCT A 934167-98-3
RGT D 121-44-8 Et3N, E 75-77-4 Me3SiCl
PRO B 934170-26-0, C 934170-27-1
SOL 107-06-2 ClCH2CH2Cl
CON 28 hours, 80 deg C

RX(3) OF 30 ...M ==> N



M

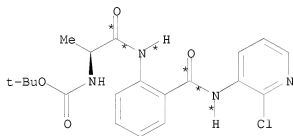
(3) →



N
YIELD 70%

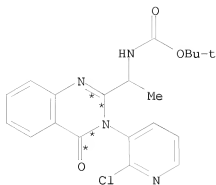
RX(3) RCT M 934167-99-4
RGT D 121-44-8 Et3N, E 75-77-4 Me3SiCl
PRO N 934170-28-2
SOL 107-06-2 ClCH2CH2Cl
CON 28 hours, 80 deg C

RX(19) OF 30 COMPOSED OF RX(9), RX(2)
RX(19) 2 A ==> B + C

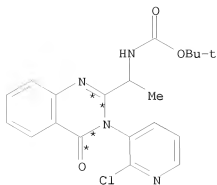


2 A

2
STEPS
→



B
YIELD 58%



C
YIELD 14%

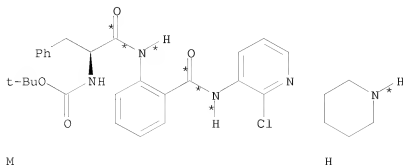
RX(9) RCT A 934167-98-3
RGT Y 7087-68-5 EtN(Pr-i)2, Z 7553-56-2 I2, AA 603-35-0 PPh3
PRO G 941569-73-9
SOL 75-09-2 CH2Cl2
CON 0.5 hours, room temperature

RX(2) RCT G 941569-73-9
STAGE(1)
RGT H 110-89-4 Piperidine
SOL 141-78-6 AcOEt
CON 15 hours, room temperature

STAGE(2)
RGT I 7646-93-7 KHSO4
SOL 7732-18-5 Water, 123-91-1 Dioxane
CON overnight, room temperature

PRO B 934170-26-0, C 934170-27-1
NTE stereoselective

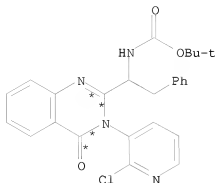
RX(28) OF 30 COMPOSED OF RX(10), RX(13), RX(4)
RX(28) M + H ==> N



M

H

3
STEPS
→



N
YIELD 100%

RX(10) RCT M 934167-99-4
RGT Y 7087-68-5 EtN(Pr-i)2, Z 7553-56-2 I2, AA 603-35-0 PPh3
PRO AB 941570-09-8
SOL 75-09-2 CH2Cl2
CON 0.5 hours, room temperature

RX(13) RCT AB 941570-09-8, H 110-89-4
PRO O 934168-01-1
SOL 141-78-6 AcOEt
CON 15 hours, room temperature

RX(4) RCT O 934168-01-1
RGT P 7631-86-9 SiO2
PRO N 934170-28-2
SOL 67-66-3 CHCl3
CON 5 days, room temperature
NTE stereoselective, silica gel used

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 26 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 146:421925 CASREACT

TITLE: Synthesis and antimicrobial activity of some sulfonamides and aryl amides

AUTHOR(S): Radadia, V. R.; Purohit, D. M.; Patolia, V. N.

CORPORATE SOURCE: Chemistry Department, Kamani Science College, Amreli, 365 601, India

SOURCE: Journal of the Institution of Chemists (India) (2006), 78(1), 8-11

CODEN: JOICA7; ISSN: 0020-3254

PUBLISHER: Institution of Chemists (India)

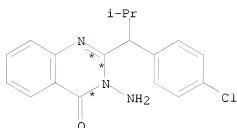
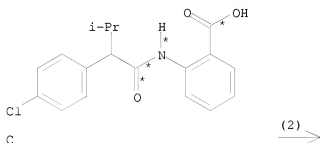
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Some new N-4-oxoquinazolin-3-yl sulfonamides and aryl amides were prepared and the constitution of the products were supported by IR, NMR, and mass

spectra. The products were screened for their antimicrobial activity compared with standard drugs. All the compds. showed moderate activity.

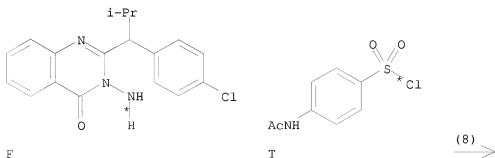
RX(2) OF 60 ...C ==> F...



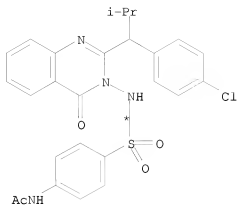
F
YIELD 86%

RX(2) RCT C 851191-19-0
 RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
 PRO F 934216-72-5
 SOL 64-17-5 EtOH
 CON 4 hours, reflux

RX(8) OF 60 ...F + T ==> U



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U
YIELD 90%

RX(8) RCT F 934216-72-5, T 121-60-8

STAGE(1)

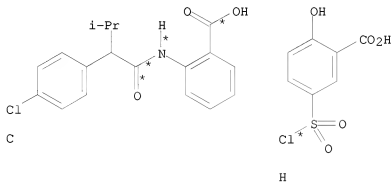
RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

STAGE(2)

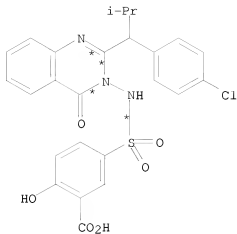
RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

PRO U 934216-78-1

RX(23) OF 60 COMPOSED OF RX(2), RX(3)
RX(23) C + H ==> I



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I
YIELD 90%

RX(2) RCT C 851191-19-0
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
PRO F 934216-72-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

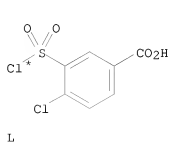
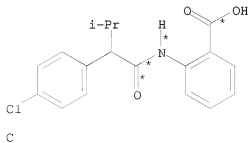
RX(3) RCT F 934216-72-5, H 17243-13-9

STAGE(1)
RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

STAGE(2)
RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

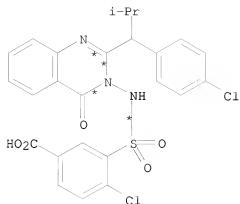
PRO I 934216-73-6

RX(24) OF 60 COMPOSED OF RX(2), RX(4)
RX(24) C + L ==> M



2
STEPS
→

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M
YIELD 90%

RX(2) RCT C 851191-19-0
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
PRO F 934216-72-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(4) RCT F 934216-72-5, L 2494-79-3

STAGE(1)

RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

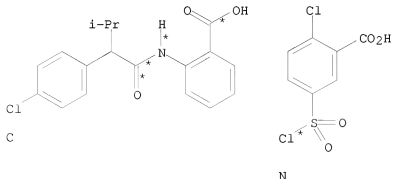
STAGE(2)

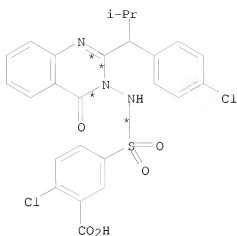
RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

PRO M 934216-74-7

RX(25) OF 60 COMPOSED OF RX(2), RX(5)

RX(25) C + N ==> O





O
YIELD 90%

RX(2) RCT C 851191-19-0
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
PRO F 934216-72-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(5) RCT F 934216-72-5, N 137-64-4

STAGE(1)

RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

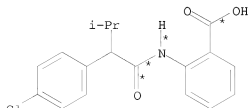
STAGE(2)

RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

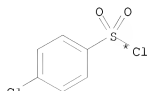
PRO O 934216-75-8

RX(26) OF 60 COMPOSED OF RX(2), RX(6)

RX(26) C + P ==> Q

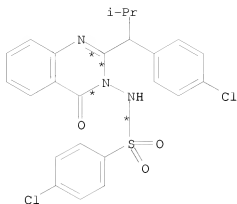


C



P

2
STEPS
→



Q

YIELD 90%

RX(2) RCT C 851191-19-0
 RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
 PRO F 934216-72-5
 SOL 64-17-5 EtOH
 CON 4 hours, reflux

RX(6) RCT F 934216-72-5, P 98-60-2

STAGE(1)

RGT D 110-86-1 Pyridine
 SOL 110-86-1 Pyridine
 CON 5 hours, reflux

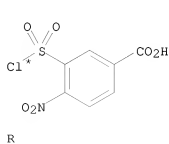
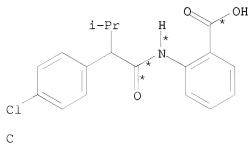
STAGE(2)

RGT J 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature, neutralized

PRO Q 934216-76-9

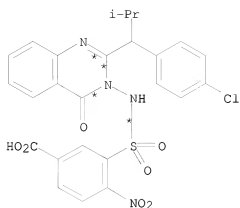
RX(27) OF 60 COMPOSED OF RX(2), RX(7)

RX(27) C + R ==> S



2
 STEPS
 →

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S

YIELD 79%

RX(2) RCT C 851191-19-0
 RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
 PRO F 934216-72-5
 SOL 64-17-5 EtOH
 CON 4 hours, reflux

RX(7) RCT F 934216-72-5, R 871243-31-1

STAGE(1)

RGT D 110-86-1 Pyridine
 SOL 110-86-1 Pyridine
 CON 5 hours, reflux

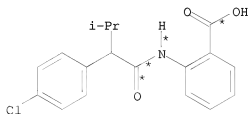
STAGE(2)

RGT J 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature, neutralized

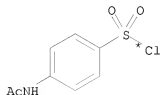
PRO S 934216-77-0

RX(28) OF 60 COMPOSED OF RX(2), RX(8)

RX(28) C + T ==> U



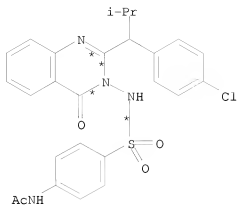
C



T

2
 STEPS
 ==>

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U
YIELD 90%

RX(2) RCT C 851191-19-0
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
PRO F 934216-72-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(8) RCT F 934216-72-5, T 121-60-8

STAGE(1)

RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

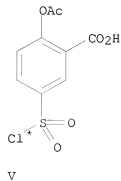
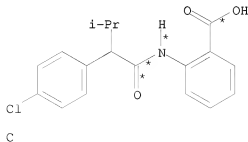
STAGE(2)

RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

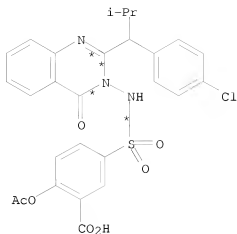
PRO U 934216-78-1

RX(29) OF 60 COMPOSED OF RX(2), RX(9)

RX(29) C + V ==> W



2
STEPS
→



W
YIELD 90%

RX(2) RCT C 851191-19-0
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
PRO F 934216-72-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

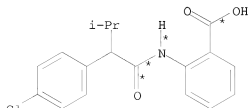
RX(9) RCT F 934216-72-5, V 77718-41-3

STAGE(1)
RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

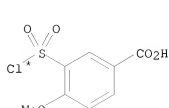
STAGE(2)
RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

PRO W 934216-79-2

RX(30) OF 60 COMPOSED OF RX(2), RX(10)
RX(30) C + X ==> Y



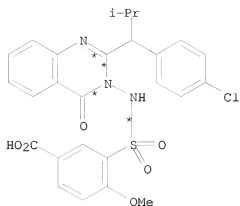
C



X

2
STEPS
→

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Y
YIELD 90%

RX(2) RCT C 851191-19-0
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
PRO F 934216-72-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(10) RCT F 934216-72-5, X 50803-29-7

STAGE(1)

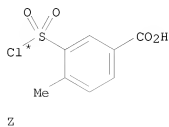
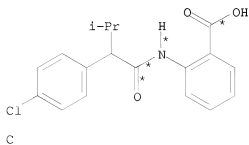
RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

STAGE(2)

RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

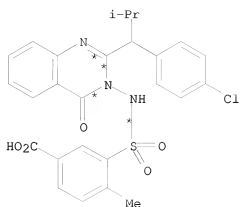
PRO Y 934216-80-5

RX(31) OF 60 COMPOSED OF RX(2), RX(11)
RX(31) C + Z ==> AA



2
STEPS
→

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AA

YIELD 90%

RX(2) RCT C 851191-19-0
 RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
 PRO F 934216-72-5
 SOL 64-17-5 EtOH
 CON 4 hours, reflux

RX(11) RCT F 934216-72-5, Z 2548-29-0

STAGE(1)

RGT D 110-86-1 Pyridine
 SOL 110-86-1 Pyridine
 CON 5 hours, reflux

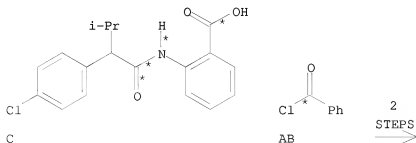
STAGE(2)

RGT J 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature, neutralized

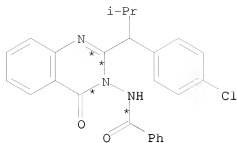
PRO AA 934216-81-6

RX(32) OF 60 COMPOSED OF RX(2), RX(12)

RX(32) C + AB ==> AC



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AC
YIELD 75%

RX(2) RCT C 851191-19-0
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
PRO F 934216-72-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

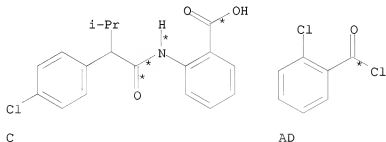
RX(12) RCT F 934216-72-5, AB 98-88-4

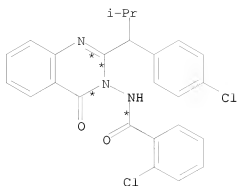
STAGE(1)
RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

STAGE(2)
RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

PRO AC 934216-82-7

RX(33) OF 60 COMPOSED OF RX(2), RX(13)
RX(33) C + AD ==> AE





AE

YIELD 75%

RX(2) RCT C 851191-19-0
 RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
 PRO F 934216-72-5
 SOL 64-17-5 EtOH
 CON 4 hours, reflux

RX(13) RCT F 934216-72-5, AD 609-65-4

STAGE(1)

RGT D 110-86-1 Pyridine
 SOL 110-86-1 Pyridine
 CON 5 hours, reflux

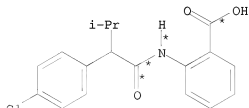
STAGE(2)

RGT J 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature, neutralized

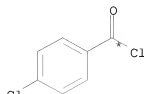
PRO AE 934216-83-8

RX(34) OF 60 COMPOSED OF RX(2), RX(14)

RX(34) C + AF ==> AG

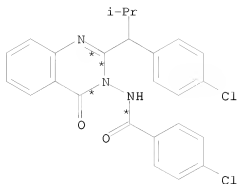


C



AF

2
 STEPS
 →



AG

YIELD 75%

RX(2) RCT C 851191-19-0
 RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
 PRO F 934216-72-5
 SOL 64-17-5 EtOH
 CON 4 hours, reflux

RX(14) RCT F 934216-72-5, AF 122-01-0

STAGE(1)

RGT D 110-86-1 Pyridine
 SOL 110-86-1 Pyridine
 CON 5 hours, reflux

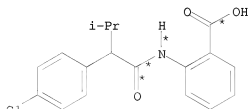
STAGE(2)

RGT J 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature, neutralized

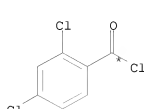
PRO AG 934216-84-9

RX(35) OF 60 COMPOSED OF RX(2), RX(15)

RX(35) C + AH ==> AI



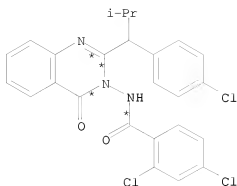
C



AH

2
 STEPS
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AI

YIELD 75%

RX(2) RCT C 851191-19-0
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
PRO F 934216-72-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(15) RCT F 934216-72-5, AH 89-75-8

STAGE(1)

RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

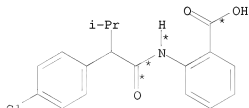
STAGE(2)

RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

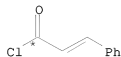
PRO AI 934216-85-0

RX(36) OF 60 COMPOSED OF RX(2), RX(16)

RX(36) C + AJ ==> AK



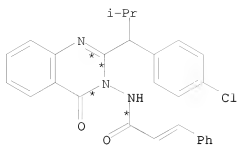
C



AJ

2
STEPS
→

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AK
YIELD 75%

RX(2) RCT C 851191-19-0
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
PRO F 934216-72-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

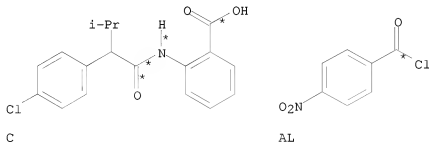
RX(16) RCT F 934216-72-5, AJ 102-92-1

STAGE(1)
RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

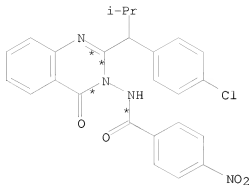
STAGE(2)
RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

PRO AK 934216-86-1

RX(37) OF 60 COMPOSED OF RX(2), RX(17)
RX(37) C + AL ==> AM



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AM

YIELD 69%

RX(2) RCT C 851191-19-0
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
PRO F 934216-72-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(17) RCT F 934216-72-5, AL 122-04-3

STAGE(1)

RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

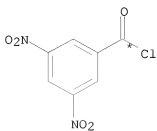
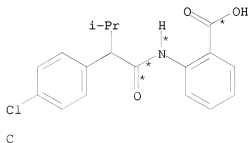
STAGE(2)

RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

PRO AM 934216-87-2

RX(38) OF 60 COMPOSED OF RX(2), RX(18)

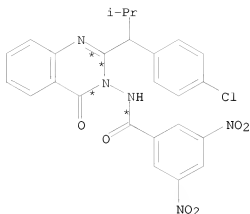
RX(38) C + AN ==> AO



AN

2
STEPS
→

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AO

YIELD 75%

RX(2) RCT C 851191-19-0
RGT G 7803-57-8 N₂H₄-H₂O, D 110-86-1 Pyridine
PRO F 934216-72-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(18) RCT F 934216-72-5, AN 99-33-2

STAGE(1)

RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

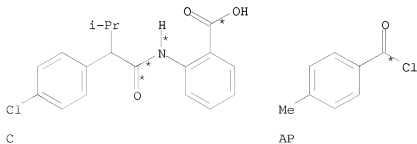
STAGE(2)

RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

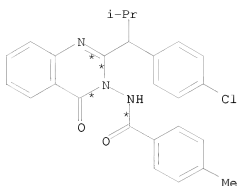
PRO AO 934216-88-3

RX(39) OF 60 COMPOSED OF RX(2), RX(19)

RX(39) C + AP ==> AQ



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AQ
YIELD 75%

RX(2) RCT C 851191-19-0
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
PRO F 934216-72-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(19) RCT F 934216-72-5, AP 874-60-2

STAGE(1)

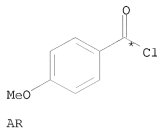
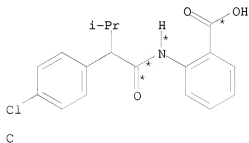
RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

STAGE(2)

RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

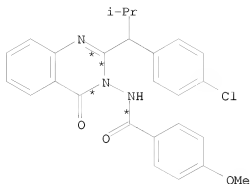
PRO AQ 934216-89-4

RX(40) OF 60 COMPOSED OF RX(2), RX(20)
RX(40) C + AR ==> AS



2
STEPS
➔

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AS

YIELD 75%

RX(2) RCT C 851191-19-0
RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
PRO F 934216-72-5
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(20) RCT F 934216-72-5, AR 100-07-2

STAGE(1)

RGT D 110-86-1 Pyridine
SOL 110-86-1 Pyridine
CON 5 hours, reflux

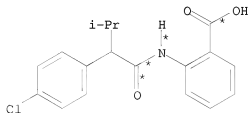
STAGE(2)

RGT J 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, neutralized

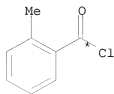
PRO AS 934216-90-7

RX(41) OF 60 COMPOSED OF RX(2), RX(21)

RX(41) C + AT ==> AU



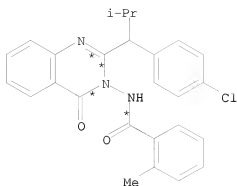
C



AT

2
STEPS
→

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AU

YIELD 75%

RX(2) RCT C 851191-19-0
 RGT G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
 PRO F 934216-72-5
 SOL 64-17-5 EtOH
 CON 4 hours, reflux

RX(21) RCT F 934216-72-5, AT 933-88-0

STAGE(1)

RGT D 110-86-1 Pyridine
 SOL 110-86-1 Pyridine
 CON 5 hours, reflux

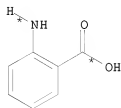
STAGE(2)

RGT J 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON room temperature, neutralized

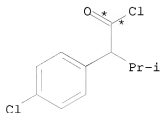
PRO AU 934216-91-8

RX(47) OF 60 COMPOSED OF RX(1), RX(2), RX(8)

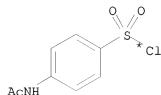
RX(47) A + B + T ==> U



A

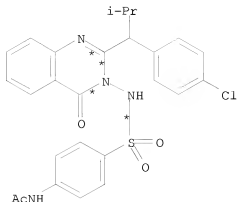


B



T

3
STEPS
→



U
YIELD 90%

```

RX(1)      RCT  A 118-92-3, B 51631-50-6
           RGT  D 110-86-1 Pyridine
           PRO  C 851191-19-0
           SOL  64-17-5 EtOH
           CON  4 hours, reflux

RX(2)      RCT  C 851191-19-0
           RGT  G 7803-57-8 N2H4-H2O, D 110-86-1 Pyridine
           PRO  F 934216-72-5
           SOL  64-17-5 EtOH
           CON  4 hours, reflux

RX(8)      RCT  F 934216-72-5, T 121-60-8

           STAGE(1)
           RGT  D 110-86-1 Pyridine
           SOL  110-86-1 Pyridine
           CON  5 hours, reflux

           STAGE(2)
           RGT  J 7647-01-0 HCl
           SOL  7732-18-5 Water
           CON  room temperature, neutralized

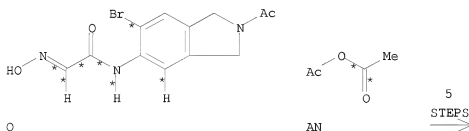
PRO  U 934216-78-1

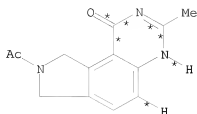
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REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 146:414392 CASREACT
 TITLE: Synthesis of dihydropyrrolo[3,4-f]quinazoline
 antifolates and their antitumor activity in vitro
 AUTHOR(S): Baek, Du-Jong
 CORPORATE SOURCE: Department of Chemistry, College of Natural Sciences,
 Sangmyung University, 7 Hongji-Dong, Chongro-Gu,
 Seoul, 110-743, S. Korea
 SOURCE: Yakhak Hoechi (2006), 50(4), 278-286
 CODEN: YAHOA3; ISSN: 0377-9556
 PUBLISHER: Pharmaceutical Society of Korea
 DOCUMENT TYPE: Journal
 LANGUAGE: Korean
 AB Classical dihydropyrrolo[3,4-f]quinazoline antifolates 7, 8 and 9, in
 which the tricyclic ring is structurally similar to the pteridine ring of
 CH2-THF (1), the cofactor of thymidylate synthase (TS), were synthesized,
 and their in vitro antitumor activity was evaluated by measuring the cell
 growth inhibitory activity against cancer cell lines. The target compds.
 were cytotoxic against CCRF-CEM, human T-cell acute lymphoblastic
 leukemia, with the cell growth inhibitory activity (IC50) of 0.8 .apprx.
 8.3 μ M. Among the three compds., 3-amino analog 7 was 10- and 3.5-fold
 more cytotoxic compared to the 3-Me analogs 8 and 9, and its cytotoxicity
 was similar to that of the reference compound with the IC50 value of 0.83 μ M.
 This result was supposed as the consequence of the fact that
 dihydropyrroloquinazolinone ring with amino group was able to bind well in
 the active site of TS. In the case of 3-Me analogs, analog 9, which has
 two-carbon bridge between the dihydropyrroloquinazolinone ring and
 benzoyl-L-glutamic acid, was 3-times more potent in cytotoxicity than
 analog 8 which has one-carbon bridge, and this result indicates that the
 distance and conformational orientation of the benzoyl-L-glutamic acid
 moiety with respect to the tricyclic ring may also be a crucial
 determinant of cell growth inhibitory activity.

RX(108) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(16)
 RX(108) Q + AN ==> AP





AP

YIELD 84%

RX(6) RCT Q 934186-17-1
 RGT H 7664-93-9 H2SO4
 PRO V 934186-18-2
 SOL 7732-18-5 Water
 CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2
 RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2
 PRO W 934186-19-3
 SOL 7732-18-5 Water
 CON 1 hour, 80 deg C

RX(8) RCT W 934186-19-3
 RGT J 1333-74-0 H2
 PRO Z 934186-20-6
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH, 109-99-9 THF
 CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7
 PRO AO 934186-27-3
 CON 4 hours, 110 deg C

RX(16) RCT AO 934186-27-3

STAGE(1)

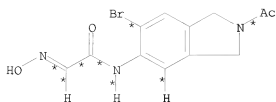
RGT AQ 7664-41-7 NH3
 CON 3 hours, -78 deg C

STAGE(2)

RGT X 1310-73-2 NaOH
 SOL 7732-18-5 Water
 CON 1 hour, reflux

PRO AP 934186-28-4

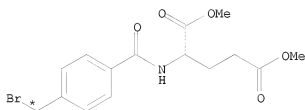
RX(109) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(18)
 RX(109) Q + AN + AK ==> AS



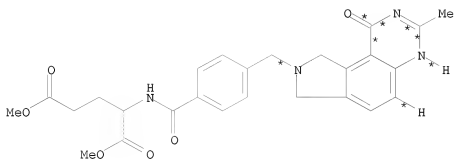
Q



AN



AK



AS

YIELD 48%

RX(6) RCT Q 934186-17-1
RGT H 7664-93-9 H2SO4
PRO V 934186-18-2
SOL 7732-18-5 Water
CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2
RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2
PRO W 934186-19-3
SOL 7732-18-5 Water
CON 1 hour, 80 deg C

RX(8) RCT W 934186-19-3
RGT J 1333-74-0 H2
PRO Z 934186-20-6
CAT 7440-05-3 Pd

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SOL 67-56-1 MeOH, 109-99-9 THF
CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7
PRO AO 934186-27-3
CON 4 hours, 110 deg C

RX(18) RCT AO 934186-27-3

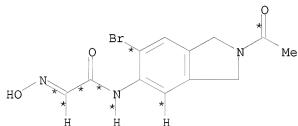
STAGE(1)
RGT D 121-44-8 Et3N
SOL 68-12-2 DMF
CON 30 minutes, room temperature

STAGE(2)
RCT AK 934186-24-0
CON 12 hours, room temperature

PRO AS 934186-30-8

RX(110) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(21)

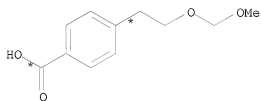
RX(110) Q + AN + AY + AZ ==> BA



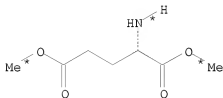
Q



AN

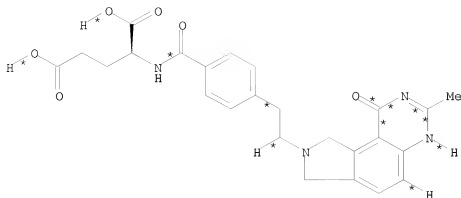


AY



AZ

5
STEPS
→



BA
YIELD 81%

RX(6) RCT Q 934186-17-1
RGT H 7664-93-9 H₂SO₄
PRO V 934186-18-2
SOL 7732-18-5 Water
CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2
RGT X 1310-73-2 NaOH, Y 7722-84-1 H₂O₂
PRO W 934186-19-3
SOL 7732-18-5 Water
CON 1 hour, 80 deg C

RX(8) RCT W 934186-19-3
RGT J 1333-74-0 H₂
PRO Z 934186-20-6
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH, 109-99-9 THF
CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7
PRO AO 934186-27-3
CON 4 hours, 110 deg C

RX(21) RCT AO 934186-27-3, AY 934186-33-1

STAGE(1)
RGT D 121-44-8 Et₃N, BB 75-75-2 MeSO₃H
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 - 5 deg C
SUBSTAGE(2) 10 minutes, 0 - 5 deg C

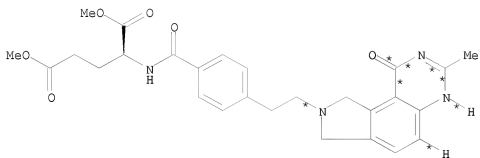
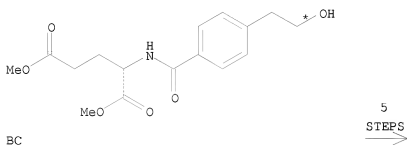
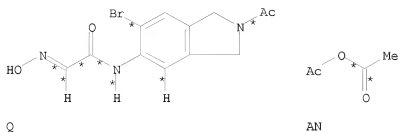
STAGE(2)
RCT AZ 6525-53-7
CON 1 hour

PRO BA 934186-31-9

RX(111) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(22)

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RX(111) Q + AN + BC ==> BD



YIELD 33%

RX(6) RCT Q 934186-17-1
RGT H 7664-93-9 H2SO4
PRO V 934186-18-2
SOL 7732-18-5 Water
CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2
RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2
PRO W 934186-19-3
SOL 7732-18-5 Water
CON 1 hour, 80 deg C

RX(8) RCT W 934186-19-3
RGT J 1333-74-0 H2

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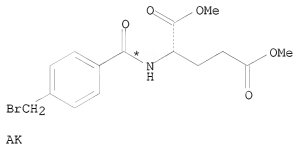
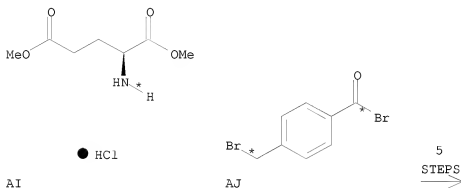
PRO Z 934186-20-6
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH, 109-99-9 THF
CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7
PRO AO 934186-27-3
CON 4 hours, 110 deg C

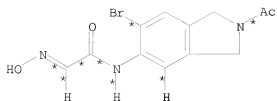
RX(22) RCT AO 934186-27-3, BC 934186-32-0
RGT AX 7087-68-5 EtN(Pr-i)2, BE 358-23-6 (F3CSO2)2O
PRO BD 934186-34-2
SOL 75-05-8 MeCN
CON 5 hours, -30 deg C

RX(133) OF 219 COMPOSED OF REACTION SEQUENCE RX(12), RX(18)
AND REACTION SEQUENCE RX(6), RX(7), RX(8), RX(15), RX(18)

...AI + AJ ==> AK...
... Q + AN + AK ==> AS



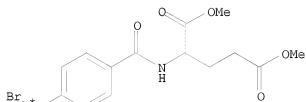
START NEXT REACTION SEQUENCE



Q

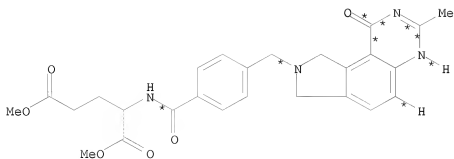


AN



AK

5
STEPS
→



AS
YIELD 48%

RX(12) RCT AI 23150-65-4

STAGE(1)

RGT D 121-44-8 Et3N
SOL 75-09-2 CH2Cl2
CON 30 minutes, 0 deg C

STAGE(2)

RCT AJ 876-07-3
CON 1 hour, 0 deg C

PRO AK 934186-24-0

RX(6) RCT Q 934186-17-1
RGT H 7664-93-9 H2SO4

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PRO V 934186-18-2
SOL 7732-18-5 Water
CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2
RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2
PRO W 934186-19-3
SOL 7732-18-5 Water
CON 1 hour, 80 deg C

RX(8) RCT W 934186-19-3
RGT J 1333-74-0 H2
PRO Z 934186-20-6
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH, 109-99-9 THF
CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7
PRO AO 934186-27-3
CON 4 hours, 110 deg C

RX(18) RCT AO 934186-27-3

STAGE(1)

RGT D 121-44-8 Et3N
SOL 68-12-2 DMF
CON 30 minutes, room temperature

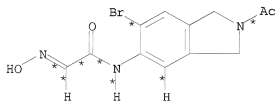
STAGE(2)

RCT AK 934186-24-0
CON 12 hours, room temperature

PRO AS 934186-30-8

RX(134) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(16), RX(17)

RX(134) Q + AN ==> AR

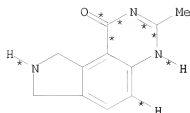


Q



AN

6
STEPS
→



● HCl

AR

YIELD 75%

RX(6) RCT Q 934186-17-1
 RGT H 7664-93-9 H2SO4
 PRO V 934186-18-2
 SOL 7732-18-5 Water
 CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2
 RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2
 PRO W 934186-19-3
 SOL 7732-18-5 Water
 CON 1 hour, 80 deg C

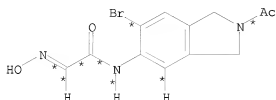
RX(8) RCT W 934186-19-3
 RGT J 1333-74-0 H2
 PRO Z 934186-20-6
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH, 109-99-9 THF
 CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7
 PRO AO 934186-27-3
 CON 4 hours, 110 deg C

RX(16) RCT AO 934186-27-3
 STAGE(1)
 RGT AQ 7664-41-7 NH3
 CON 3 hours, -78 deg C
 STAGE(2)
 RGT X 1310-73-2 NaOH
 SOL 7732-18-5 Water
 CON 1 hour, reflux
 PRO AP 934186-28-4

RX(17) RCT AP 934186-28-4
 RGT S 7647-01-0 HCl
 PRO AR 934186-29-5
 SOL 7732-18-5 Water
 CON 12 hours, reflux

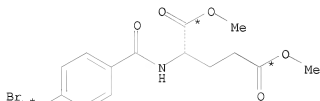
RX(135) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(18), RX(19)
 RX(135) Q + AN + AK ==> AT



Q

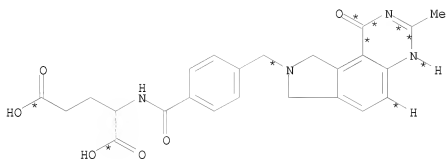


AN



AK

6
 STEPS
 ➞



AT
 YIELD 71%

RX(6) RCT Q 934186-17-1
 RGT H 7664-93-9 H2SO4
 PRO V 934186-18-2
 SOL 7732-18-5 Water
 CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2
 RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2
 PRO W 934186-19-3
 SOL 7732-18-5 Water
 CON 1 hour, 80 deg C

10/ 562,112

RX(8) RCT W 934186-19-3
RGT J 1333-74-0 H2
PRO Z 934186-20-6
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH, 109-99-9 THF
CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7
PRO AO 934186-27-3
CON 4 hours, 110 deg C

RX(18) RCT AO 934186-27-3

STAGE(1)

RGT D 121-44-8 Et3N
SOL 68-12-2 DMF
CON 30 minutes, room temperature

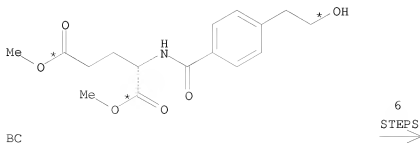
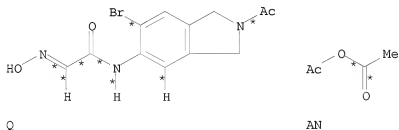
STAGE(2)

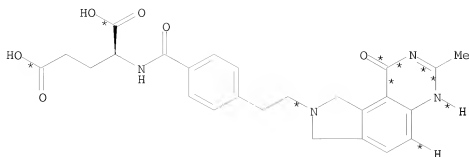
RCT AK 934186-24-0
CON 12 hours, room temperature

PRO AS 934186-30-8

RX(19) RCT AS 934186-30-8
RGT X 1310-73-2 NaOH
PRO AT 934186-26-2
SOL 7732-18-5 Water
CON 3 hours, 60 deg C

RX(136) OF 219 COMPOSED OF RX(6), RX(7), RX(8), RX(15), RX(22), RX(23)
RX(136) Q + AN + BC ==> BA





BA
YIELD 59%

RX(6) RCT Q 934186-17-1
RGT H 7664-93-9 H2SO4
PRO V 934186-18-2
SOL 7732-18-5 Water
CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2
RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2
PRO W 934186-19-3
SOL 7732-18-5 Water
CON 1 hour, 80 deg C

RX(8) RCT W 934186-19-3
RGT J 1333-74-0 H2
PRO Z 934186-20-6
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH, 109-99-9 THF
CON 2 hours, room temperature

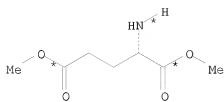
RX(15) RCT Z 934186-20-6, AN 108-24-7
PRO AO 934186-27-3
CON 4 hours, 110 deg C

RX(22) RCT AO 934186-27-3, BC 934186-32-0
RGT AX 7087-68-5 EtN(Pr-i)2, BE 358-23-6 (F3CSO2)2O
PRO BD 934186-34-2
SOL 75-05-8 MeCN
CON 5 hours, -30 deg C

RX(23) RCT BD 934186-34-2
RGT X 1310-73-2 NaOH
PRO BA 934186-31-9
SOL 7732-18-5 Water
CON 3 hours, 60 deg C

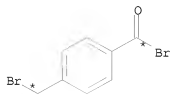
RX(166) OF 219 COMPOSED OF REACTION SEQUENCE RX(12), RX(18), RX(19)
AND REACTION SEQUENCE RX(6), RX(7), RX(8), RX(15), RX(18),
RX(19)

...AI + AJ ==> AK...
... Q + AN + AK ==> AT

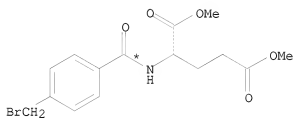


● HCl

AI

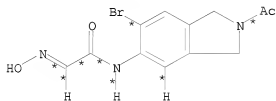


AJ

6
STEPS
→

AK

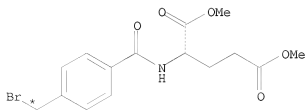
START NEXT REACTION SEQUENCE



Q

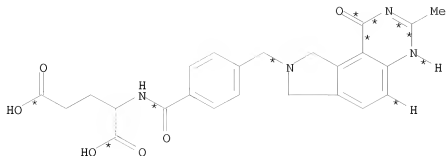


AN



AK

6
STEPS
→



AT
YIELD 71%

RX(12) RCT AI 23150-65-4

STAGE(1)

RGT D 121-44-8 Et3N
SOL 75-09-2 CH2Cl2
CON 30 minutes, 0 deg C

STAGE(2)

RGT AJ 876-07-3
CON 1 hour, 0 deg C

PRO AK 934186-24-0

RX(6) RCT Q 934186-17-1
RGT H 7664-93-9 H2SO4
PRO V 934186-18-2
SOL 7732-18-5 Water
CON 2 hours, 80 deg C

RX(7) RCT V 934186-18-2
RGT X 1310-73-2 NaOH, Y 7722-84-1 H2O2
PRO W 934186-19-3
SOL 7732-18-5 Water
CON 1 hour, 80 deg C

RX(8) RCT W 934186-19-3
RGT J 1333-74-0 H2
PRO Z 934186-20-6
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH, 109-99-9 THF
CON 2 hours, room temperature

RX(15) RCT Z 934186-20-6, AN 108-24-7
PRO AO 934186-27-3
CON 4 hours, 110 deg C

RX(18) RCT AO 934186-27-3

STAGE(1)

RGT D 121-44-8 Et3N
SOL 68-12-2 DMF
CON 30 minutes, room temperature

STAGE(2)

RCT AK 934186-24-0

CON 12 hours, room temperature

PRO AS 934186-30-8

RX(19) RCT AS 934186-30-8
 RGT X 1310-73-2 NaOH
 PRO AT 934186-26-2
 SOL 7732-18-5 Water
 CON 3 hours, 60 deg C

L3 ANSWER 28 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 146:337611 CASREACT

TITLE: Kynurenic acid amides as novel NR2B selective NMDA receptor antagonists

AUTHOR(S): Borza, Istvan; Kolok, Sandor; Galgoczy, Kornel; Gere, Aniko; Horvath, Csilla; Farkas, Sandor; Greiner, Istvan; Domany, Gyoergy

CORPORATE SOURCE: Gedeon Richter Ltd., H-1475, Hung.

SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(2), 406-409

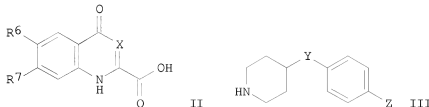
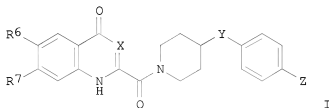
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

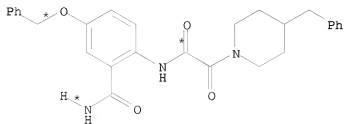
GI



AB A novel series of kynurenic acid amides I ($R_6 = H, OH, MeCONH$, $R_7 = H, OH$, $R_6R_7 = NHC(O)O$, $X = CH, NH$, $Y = CH_2, O$, $Z = H, F, Cl, Me$), ring-enlarged derivs. of indole-2-carboxamides, was prepared and identified as in vivo active NR2B subtype selective NMDA receptor antagonists. The synthesis

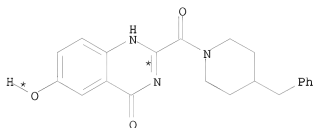
and SAR studies are discussed. The key step in the synthesis was a standard coupling reaction between and appropriately substituted kynurenic acid II and a piperidine III.

RX(27) OF 72 ...BF ==> BG



BF

(27)



BG

RX(27) RCT BF 929028-80-8

STAGE(1)

CON 1.5 hours, 250 deg C

STAGE(2)

RGT N 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 109-99-9 THF

CON room temperature

PRO BG 929028-81-9

NTE thermal (stage 1)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

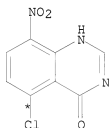
L3 ANSWER 29 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 146:45478 CASREACT

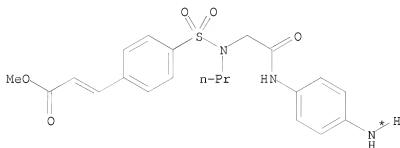
TITLE: 4'-Alkoxy substitution enhancing the anti-mitotic effect of 5-(3',4',5'-substituted)anilino-4-hydroxy-8-nitroquinazolines as a novel class of anti-microtubule

agents
 AUTHOR(S): Jin, Yi; Zhou, Zu-Yu; Tian, Wei; Yu, Qiang; Long, Ya-Qiu
 CORPORATE SOURCE: State Key Laboratory of Drug Research, Shanghai
 Institute of Materia Medica, Shanghai Institutes for
 Biological Sciences, Chinese Academy of Sciences,
 Shanghai, 201203, Peop. Rep. China
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),
 16(22), 5864-5869
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Mitosis inhibitors are powerful anticancer drugs. Based on a novel
 anti-microtubule agent 5-(4'-methoxy)anilino-4-hydroxy-8-nitroquinazoline,
 a series of 5-(3',4',5'-substituted)anilino-4-hydroxy-8-nitroquinazolines
 were designed and synthesized to investigate the effect of the
 substitution on the inhibitory activity against mitotic progression of
 tumor cells. The large alkoxy substitution on the 4'-position of
 5-anilino ring is beneficial for the potency. The
 5-(3',4',5'-trimethoxy)anilino-8-nitroquinazoline (1h) displays an
 overwhelming activity in arresting the cells at the G2/M phase, providing
 a promising new template for further development of potent
 microtubule-targeted anti-mitotic drugs.

RX(35) OF 146 ...CB + AY ==> CG

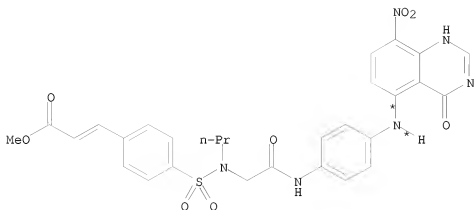


CB



AY

(35)
 →



CG

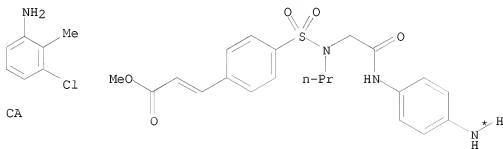
YIELD 80%

RX(19) RCT AP 916336-31-7
 RGT O 12125-02-9 NH₄Cl, P 7439-89-6 Fe
 PRO AY 916336-22-6
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON reflux

RX(35) RCT CB 400784-50-1, AY 916336-22-6
 RGT AN 7087-68-5 EtN(Pr-i)₂
 PRO CG 916336-26-0
 SOL 109-99-9 THF
 CON 12 - 24 hours, reflux

RX(72) OF 146 COMPOSED OF RX(30), RX(35)

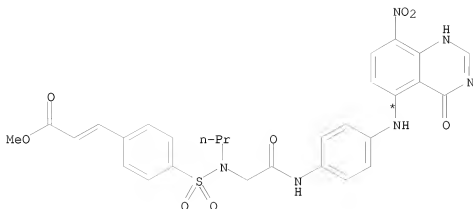
RX(72) CA + AY ==> CG



CA

AY

2
 STEPS
 →

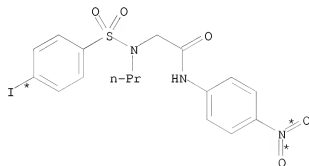
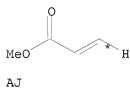


CG
YIELD 80%

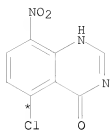
RX(30) RCT CA 87-60-5
PRO CB 400784-50-1
NTE no experimental detail

RX(35) RCT CB 400784-50-1, AY 916336-22-6
RGT AN 7087-68-5 EtN(Pr-i)₂
PRO CG 916336-26-0
SOL 109-99-9 THF
CON 12 - 24 hours, reflux

RX(98) OF 146 COMPOSED OF RX(14), RX(19), RX(35)
RX(98) AJ + AO + CB ==> CG

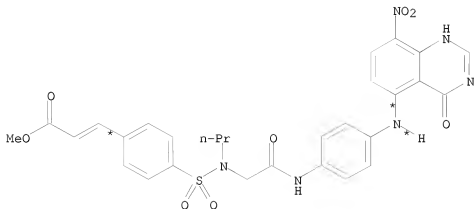


AO



CB

3
STEPS
→



CG

YIELD 80%

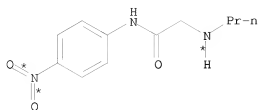
RX(14) RCT AJ 96-33-3, AO 916336-34-0
 RGT AL 7699-45-8 ZnBr₂
 PRO AP 916336-31-7
 CAT 13965-03-2 PdCl₂(PPh₃)₂
 SOL 109-99-9 THF, 7087-68-5 EtN(Pr-i)₂
 CON room temperature

RX(19) RCT AP 916336-31-7
 RGT O 12125-02-9 NH₄Cl, P 7439-89-6 Fe
 PRO AY 916336-22-6
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON reflux

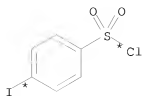
RX(35) RCT CB 400784-50-1, AY 916336-22-6
 RGT AN 7087-68-5 EtN(Pr-i)₂
 PRO CG 916336-26-0
 SOL 109-99-9 THF
 CON 12 - 24 hours, reflux

RX(99) OF 146 COMPOSED OF RX(18), RX(14), RX(19), RX(35)
 RX(99) AW + AX + AJ + CB ==> CG

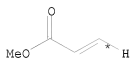
10/ 562,112



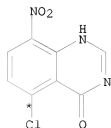
AW



AX

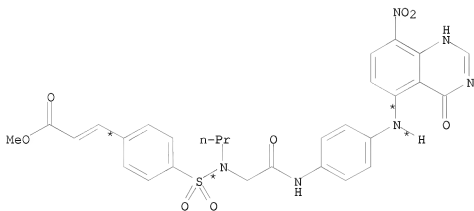


AJ



CB

4
STEPS
→



CG

YIELD 80%

RX(18) RCT AW 699532-45-1, AX 98-61-3
RGT AN 7087-68-5 EtN(Pr-i)2
PRO AO 916336-34-0
SOL 109-99-9 THF
CON room temperature

RX(14) RCT AJ 96-33-3, AO 916336-34-0
RGT AL 7699-45-8 ZnBr2
PRO AP 916336-31-7
CAT 13965-03-2 PdCl2(PPh3)2

SOL 109-99-9 THF, 7087-68-5 EtN(Pr-i)2
 CON room temperature

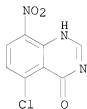
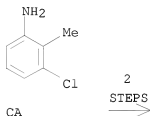
RX(19) RCT AP 916336-31-7
 RGT O 12125-02-9 NH4Cl, P 7439-89-6 Fe
 PRO AY 916336-22-6
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON reflux

RX(35) RCT CB 400784-50-1, AY 916336-22-6
 RGT AN 7087-68-5 EtN(Pr-i)2
 PRO CG 916336-26-0
 SOL 109-99-9 THF
 CON 12 - 24 hours, reflux

RX(107) OF 146 COMPOSED OF REACTION SEQUENCE RX(30), RX(35)
 AND REACTION SEQUENCE RX(19), RX(35)

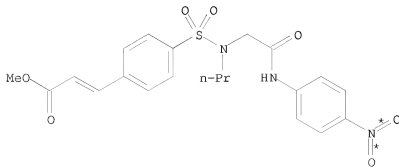
...CA ==> CB...

... AP + CB ==> CG

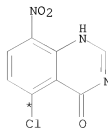


CB

START NEXT REACTION SEQUENCE

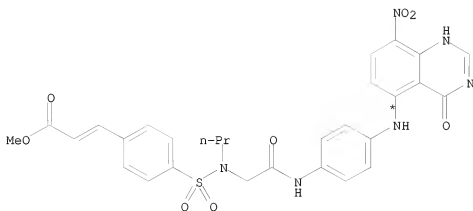


AP



CB

2
STEPS
→



CG
YIELD 80%

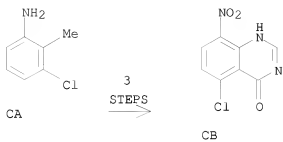
RX(30) RCT CA 87-60-5
PRO CB 400784-50-1
NTE no experimental detail

RX(19) RCT AP 916336-31-7
RGT O 12125-02-9 NH4Cl, P 7439-89-6 Fe
PRO AY 916336-22-6
SOL 7732-18-5 Water, 67-56-1 MeOH
CON reflux

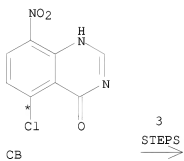
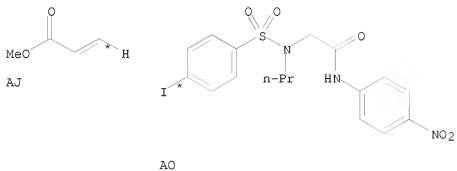
RX(35) RCT CB 400784-50-1, AY 916336-22-6
RGT AN 7087-68-5 EtN(Pr-i)2
PRO CG 916336-26-0
SOL 109-99-9 THF
CON 12 - 24 hours, reflux

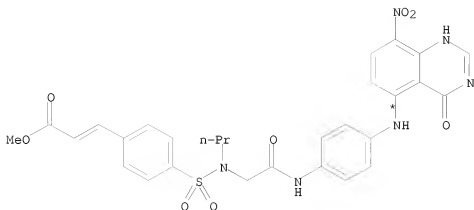
RX(108) OF 146 COMPOSED OF REACTION SEQUENCE RX(30), RX(35)
AND REACTION SEQUENCE RX(14), RX(19), RX(35)

...CA ==> CB...
...AJ + AO + CB ==> CG



START NEXT REACTION SEQUENCE





CG

YIELD 80%

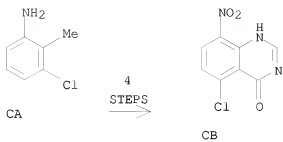
RX(30) RCT CA 87-60-5
 PRO CB 400784-50-1
 NIE no experimental detail

RX(14) RCT AJ 96-33-3, AO 916336-34-0
 RGT AL 7699-45-8 ZnBr2
 PRO AP 916336-31-7
 CAT 13965-03-2 PdCl2(PPh3)2
 SOL 109-99-9 THF, 7087-68-5 EtN(Pr-i)2
 CON room temperature

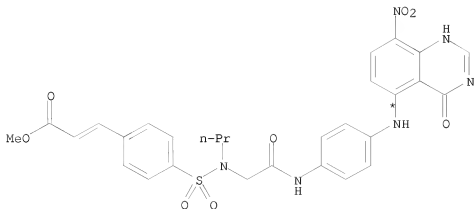
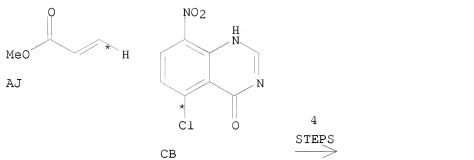
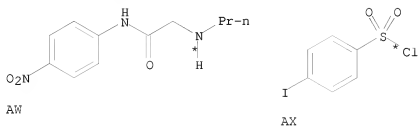
RX(19) RCT AP 916336-31-7
 RGT O 12125-02-9 NH4Cl, P 7439-89-6 Fe
 PRO AY 916336-22-6
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON reflux

RX(35) RCT CB 400784-50-1, AY 916336-22-6
 RGT AN 7087-68-5 EtN(Pr-i)2
 PRO CG 916336-26-0
 SOL 109-99-9 THF
 CON 12 - 24 hours, reflux

RX(135) OF 146 COMPOSED OF REACTION SEQUENCE RX(30), RX(35)
 AND REACTION SEQUENCE RX(18), RX(14), RX(19), RX(35)
 ...CA ==> CB...
 ... AW + AX + AJ + CB ==> CG



START NEXT REACTION SEQUENCE



YIELD 80%

RX(30) RCT CA 87-60-5
 PRO CB 400784-50-1
 NTE no experimental detail

 RX(18) RCT AW 699532-45-1, AX 98-61-3
 RGT AN 7087-68-5 EtN(Pr-i)2
 PRO AO 916336-34-0
 SOL 109-99-9 THF
 CON room temperature

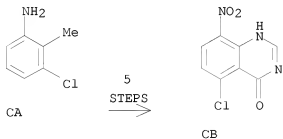
 RX(14) RCT AJ 96-33-3, AO 916336-34-0
 RGT AL 7699-45-8 ZnBr2
 PRO AP 916336-31-7
 CAT 13965-03-2 PdCl2(PPh3)2
 SOL 109-99-9 THF, 7087-68-5 EtN(Pr-i)2
 CON room temperature

 RX(19) RCT AP 916336-31-7
 RGT O 12125-02-9 NH4Cl, P 7439-89-6 Fe
 PRO AY 916336-22-6
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON reflux

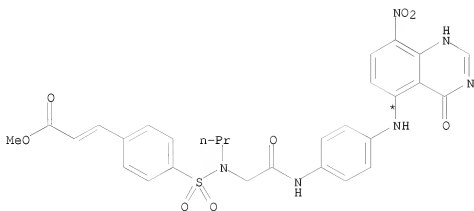
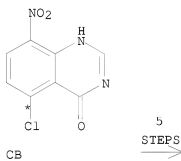
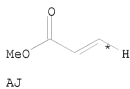
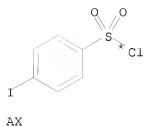
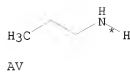
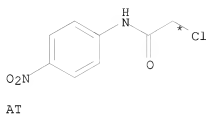
 RX(35) RCT CB 400784-50-1, AY 916336-22-6
 RGT AN 7087-68-5 EtN(Pr-i)2
 PRO CG 916336-26-0
 SOL 109-99-9 THF
 CON 12 - 24 hours, reflux

RX(136) OF 146 COMPOSED OF REACTION SEQUENCE RX(30), RX(35)
 AND REACTION SEQUENCE RX(17), RX(18), RX(14), RX(19), RX(35)

...CA ==> CB...
 ... AT + AV + AX + AJ + CB ==> CG



START NEXT REACTION SEQUENCE



CG
YIELD 80%

RX(30) RCT CA 87-60-5
 PRO CB 400784-50-1

NTE no experimental detail

RX(17) RCT AT 17329-87-2, AV 107-10-8
 PRO AW 699532-45-1
 SOL 109-99-9 THF
 CON room temperature

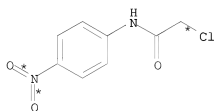
RX(18) RCT AW 699532-45-1, AX 98-61-3
 RGT AN 7087-68-5 EtN(Pr-i)2
 PRO AO 916336-34-0
 SOL 109-99-9 THF
 CON room temperature

RX(14) RCT AJ 96-33-3, AO 916336-34-0
 RGT AL 7699-45-8 ZnBr2
 PRO AP 916336-31-7
 CAT 13965-03-2 PdCl2(PPh3)2
 SOL 109-99-9 THF, 7087-68-5 EtN(Pr-i)2
 CON room temperature

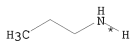
RX(19) RCT AP 916336-31-7
 RGT O 12125-02-9 NH4Cl, P 7439-89-6 Fe
 PRO AY 916336-22-6
 SOL 7732-18-5 Water, 67-56-1 MeOH
 CON reflux

RX(35) RCT CB 400784-50-1, AY 916336-22-6
 RGT AN 7087-68-5 EtN(Pr-i)2
 PRO CG 916336-26-0
 SOL 109-99-9 THF
 CON 12 - 24 hours, reflux

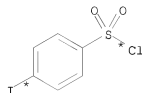
RX(139) OF 146 COMPOSED OF RX(17), RX(18), RX(14), RX(19), RX(35)
 RX(139) AT + AV + AX + AJ + CB ==> CG



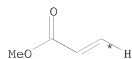
AT



AV



AX

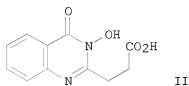
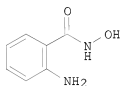


AJ

RX(35) RCT CB 400784-50-1, AY 916336-22-6
 RGT AN 7087-68-5 EtN(Pr-i)2
 PRO CG 916336-26-0
 SOL 109-99-9 THF
 CON 12 - 24 hours, reflux

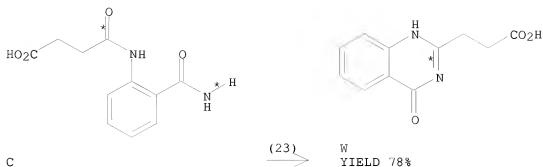
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 30 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 145:505395 CASREACT
 TITLE: Reaction of anthranilic acid amides with cyclic
 anhydrides
 AUTHOR(S): Shemchuk, L. A.; Chernykh, V. P.; Krys'kiv, O. S.
 CORPORATE SOURCE: National Pharmaceutical University, Kharkov, 61002,
 Ukraine
 SOURCE: Russian Journal of Organic Chemistry (2006), 42(3),
 382-387
 CODEN: RJOCEQ; ISSN: 1070-4280
 PUBLISHER: Pleiades Publishing, Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



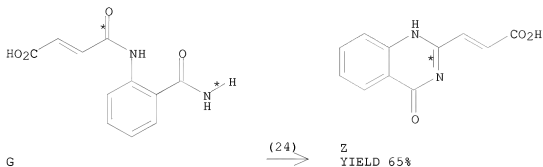
AB Anthranilic acid amide reacts with cyclic anhydrides to give the
 corresponding N-acyl derivs. at the amino group, while analogous reactions
 of o-aminobenzohydroxamic acid (I) lead to formation of
 3-hydroxy-quinazolin-4-ones, e.g., II, under mild conditions. N-Acyl
 derivs. of anthranilic acid amide undergo intramol. cyclization to imides
 on microwave irradiation or on melting, and their treatment with acetic
 anhydride in the presence of sodium acetate on heating yields
 quinazolin-4-ones.

RX(23) OF 56 ...C ==> W...



RX(23) RCT C 306325-56-4
 RGT X 127-09-3 AcONa
 PRO W 5368-37-6
 SOL 108-24-7 Ac2O
 CON SUBSTAGE(1) 15 minutes, reflux
 SUBSTAGE(2) cooled
 NTE products depend on reaction conditions

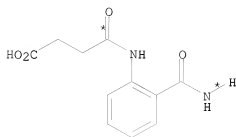
RX(24) OF 56 ...G ==> Z...



RX(24) RCT G 303770-83-4
 RGT X 127-09-3 AcONa
 PRO Z 5584-96-3
 SOL 108-24-7 Ac2O
 CON SUBSTAGE(1) 15 minutes, reflux
 SUBSTAGE(2) cooled
 NTE products depend on reaction conditions

RX(51) OF 56 COMPOSED OF RX(23), RX(30)
 RX(51) C + AE ==> AF

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C



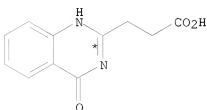
AE

2
STEPS
→



AF: CM 1

YIELD 77%



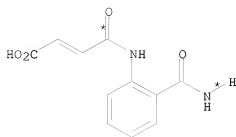
AF: CM 2

YIELD 77%

RX(23) RCT C 306325-56-4
RGT X 127-09-3 AcONa
PRO W 5368-37-6
SOL 108-24-7 Ac2O
CON SUBSTAGE(1) 15 minutes, reflux
SUBSTAGE(2) cooled
NTE products depend on reaction conditions

RX(30) RCT W 5368-37-6, AE 100-46-9
PRO AF 915215-79-1
SOL 64-17-5 EtOH
CON 30 minutes, room temperature
NTE using dioxane as solvent gave same result

RX(52) OF 56 COMPOSED OF RX(24), RX(31)
RX(52) G + AE ==> AH



G

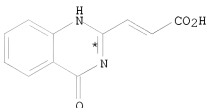


AE

2
STEPS
→



AH: CM 1
YIELD 65%



AH: CM 2
YIELD 65%

RX(24) RCT G 303770-83-4
RGT X 127-09-3 AcONa
PRO Z 5584-96-3
SOL 108-24-7 Ac2O
CON SUBSTAGE(1) 15 minutes, reflux
SUBSTAGE(2) cooled
NTE products depend on reaction conditions

RX(31) RCT Z 5584-96-3, AE 100-46-9
PRO AH 915215-80-4
SOL 64-17-5 EtOH
CON 30 minutes, room temperature
NTE using dioxane as solvent gave same result

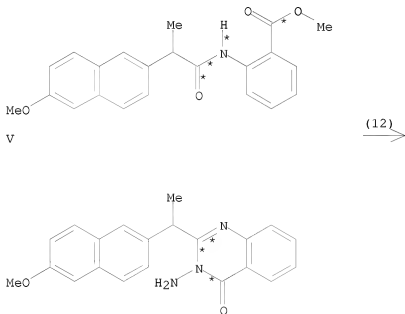
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 31 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 145:489192 CASREACT
TITLE: Propionic acids in organic synthesis: novel synthesis of benzimidazole, 3,1-benzoxazine, 3-aminoquinazoline and 3-aminothieno[2,3-d]pyrimidine derivatives containing 2-naphthyl propionyl moiety
AUTHOR(S): Al-Sehemi, Abdullah G. M.; El-Sharief, A. M. Sh; Ammar, Y. A.
CORPORATE SOURCE: Chemistry Department, Teacher's College, Abha, Saudi

SOURCE: Arabia
 Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (2006),
 45B(2), 450-455
 CODEN: IJSBDB; ISSN: 0376-4699
 PUBLISHER: National Institute of Science Communication and
 Information Resources
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Naproxenoyl chloride (I) is reacted with NH_4SCN and NaN_3 to produce the acid isothiocyanate and acid azide, resp. Interaction of the isothiocyanate with 1,2-phenylenediamine and anthranilic acid produced the corresponding benzimidazole 5 and 3,1-benzoxazine, resp. Treatment of the acid azide with 4-toluidine afforded the corresponding urea derivative A novel quinazolinone is synthesized by acylation of Me anthranilate with I followed by treatment with $\text{N}_2\text{H}_4\cdot\text{H}_2\text{O}$.

RX(12) OF 65 ...V ==> AA...

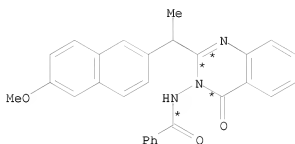
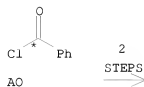
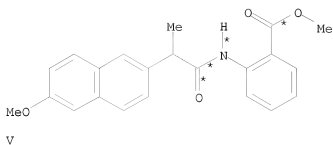


AA
 YIELD 65%

RX(12) RCT V 177585-58-9
 RGT AB 7803-57-8 $\text{N}_2\text{H}_4\cdot\text{H}_2\text{O}$
 PRO AA 354786-03-1
 SOL 71-36-3 BuOH
 CON 10 hours, reflux

RX(42) OF 65 COMPOSED OF RX(12), RX(20)
 RX(42) V + AO ==> AP

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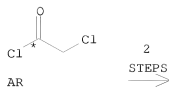
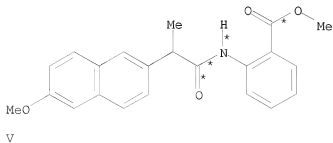
YIELD 60%

RX(12) RCT V 177585-58-9
RGT AB 7803-57-8 N2H4-H2O
PRO AA 354786-03-1
SOL 71-36-3 BuOH
CON 10 hours, reflux

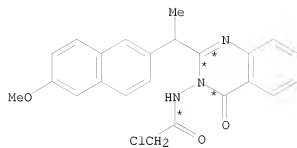
RX(20) RCT AA 354786-03-1, AO 98-88-4
RGT AQ 110-86-1 Pyridine
PRO AP 914398-10-0
SOL 110-86-1 Pyridine
CON 1 hour, reflux

RX(43) OF 65 COMPOSED OF RX(12), RX(21)

RX(43) V + AR ==> AS



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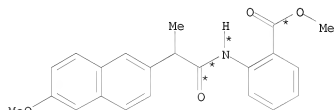


AS
YIELD 62%

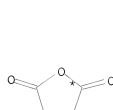
RX(12) RCT V 177585-58-9
RGT AB 7803-57-8 N2H4-H2O
PRO AA 354786-03-1
SOL 71-36-3 BuOH
CON 10 hours, reflux

RX(21) RCT AA 354786-03-1, AR 79-04-9
RGT AQ 110-86-1 Pyridine
PRO AS 914398-11-1
SOL 110-86-1 Pyridine
CON 1 hour, reflux

RX(44) OF 65 COMPOSED OF RX(12), RX(22)
RX(44) V + AT ==> AU



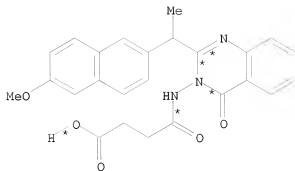
V



AT

2
STEPS
→

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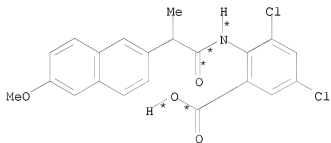


AU
YIELD 60%

RX(12) RCT V 177585-58-9
RGT AB 7803-57-8 N2H4-H2O
PRO AA 354786-03-1
SOL 71-36-3 BuOH
CON 10 hours, reflux

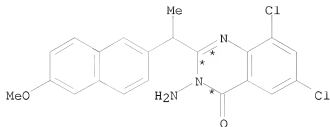
RX(22) RCT AA 354786-03-1, AT 108-30-5
PRO AU 914398-12-2
SOL 64-17-5 EtOH
CON 3 hours, reflux

RX(45) OF 65 COMPOSED OF RX(14), RX(15)
RX(45) Z ==> AG



Z

2
STEPS
→



AG
YIELD 62%

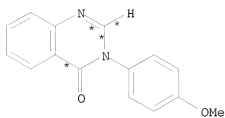
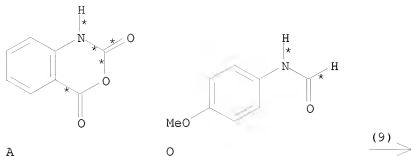
RX(14) RCT Z 914398-03-1
RGT AE 108-24-7 Ac2O
PRO AF 914398-05-3
SOL 108-24-7 Ac2O
CON 5 hours, reflux

RX(15) RCT AF 914398-05-3
RGT AB 7803-57-8 N2H4-H2O
PRO AG 914398-22-4
SOL 64-17-5 EtOH
CON 24 hours, reflux

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 32 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 145:271726 CASREACT
TITLE: Convergent one-pot synthesis of 3-substituted quinazolin-4(3H)-ones under solvent-free conditions
AUTHOR(S): Samavi, Laleh
CORPORATE SOURCE: Department of Chemistry, Guilan University, Rasht, Iran
SOURCE: Synthetic Communications (2006), 36(15), 2245-2252
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Taylor & Francis, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A convenient method for the synthesis of 3-substituted quinazolin-4(3H)-ones using the convergent reactions of formic acid, a primary amine, and isatoic anhydride under solvent-free conditions and with brief microwave irradiation is described.

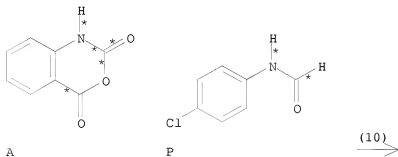
RX(9) OF 18 ...A + O ==> L

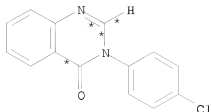


L
YIELD 62%

RX(9) RCT A 118-48-9, O 5470-34-8
 PRO L 22378-45-6
 CON 6 minutes, heated
 NIE a few drops of DMF used, green chemistry-solvent, microwave
 irradiation, no solvent

RX(10) OF 18 ...A + P ==> N



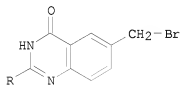


N
YIELD 71%

RX(10) RCT A 118-48-9, P 2617-79-0
PRO N 24122-31-4
CON 6 minutes, heated
NTE a few drops of DMF used, green chemistry-solvent, microwave irradiation, no solvent

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 33 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 145:230582 CASREACT
TITLE: Syntheses of 2-substituted
6-bromomethyl-4(3H)-quinazolinones
AUTHOR(S): Cao, Sheng-Li; Feng, Yu-Ping; Gao, Hong-He; Feng, Ke-Ran
CORPORATE SOURCE: Department of Chemistry, Capital Normal University, Beijing, 100037, Peop. Rep. China
SOURCE: Yingyong Huaxue (2005), 22(9), 1027-1029
CODEN: YIHUED; ISSN: 1000-0518
PUBLISHER: Kexue Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI

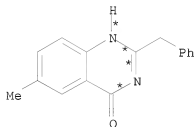
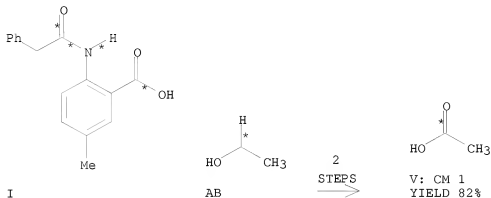


AB 2-Amino-5-methylbenzoic acid (I) was acylated with acyl chlorides, then heated with acetic anhydride to give 2-Ph or 2-benzyl-6-methylbenzoxazin-4-one, while I was reacted with propanoic anhydride or trifluoroacetic anhydride to give 2-Et or 2-trifluoromethyl-6-methyl-benzoxazin-4-one directly. Then, 2-substituted 6-methylbenzoxazin-4-ones were heated with formamide to afford 2-substituted 6-methyl-4(3H)-quinazolinones, which were converted into the title compds. II (R = Ph, CH2Ph, CH2CH3, CF3) via bromination with

N-bromosuccinimide in the presence of (PhCOO)₂. The structures of all the intermediates and final products were confirmed with ESI-MS, ¹H-NMR and elemental anal.

RX(18) OF 32 COMPOSED OF RX(4), RX(12)

RX(18) I + AB ==> V



V: CM 2
YIELD 82%

RX(4) RCT I 157834-20-3
RGT K 108-24-7 Ac2O
PRO L 157834-12-3
CON 3 hours, reflux

RX(12) RCT L 157834-12-3

STAGE(1)

RGT AC 75-12-7 Formamide
CON 3 hours, 150 - 155 deg C

STAGE(2)

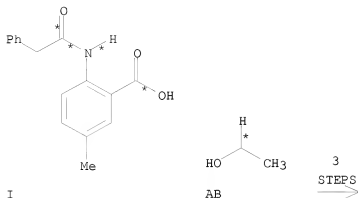
RGT AB 64-17-5
SOL 7732-18-5 Water

PRO V 905455-25-6

RX(29) OF 32 COMPOSED OF RX(4), RX(12), RX(8)

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RX(29) I + AB ==> W



W
YIELD 44%

RX(4) RCT I 157834-20-3
RGT K 108-24-7 Ac2O
PRO L 157834-12-3
CON 3 hours, reflux

RX(12) RCT L 157834-12-3

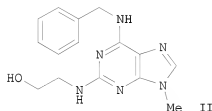
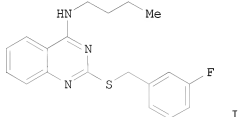
STAGE(1)
RGT AC 75-12-7 Formamide
CON 3 hours, 150 - 155 deg C

STAGE(2)
RCT AB 64-17-5
SOL 7732-18-5 Water

PRO V 905455-25-6

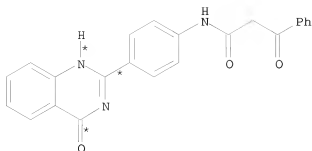
RX(8) RCT V 905455-25-6
RGT S 94-36-0 Benzoyl peroxide, T 128-08-5 Bromosuccinimide
PRO W 905455-23-4
SOL 67-66-3 CHCl3
CON 3 hours, reflux

L3 ANSWER 34 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 145:124518 CASREACT
 TITLE: An efficient direct amination of cyclic amides and cyclic ureas
 AUTHOR(S): Wan, Zhao-Kui; Wacharasindhu, Sumrit; Binnun, Eva; Mansour, Tarek
 CORPORATE SOURCE: Chemical and Screening Sciences, Wyeth Research, Cambridge, MA, 02140, USA
 SOURCE: Organic Letters (2006), 8(11), 2425-2428
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB An efficient one-step amination of cyclic amides and ureas has been developed. Treatment of cyclic amides and cyclic ureas with BOP in the presence of DBU in various solvents led to the formation of cyclic amidines and cyclic guanidines, e.g., I, in good to excellent yields. Concise syntheses of biol. intriguing kinetin and potent kinase inhibitor olomoucine (II) were thus achieved in just one and two steps, resp.

RX(21) OF 40 AB + AS ==> AT

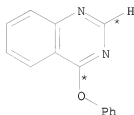


AB



AS

(21) →



AT

YIELD 84%

RX(21) RCT AB 95812-45-6

STAGE(1)

RGT D 6674-22-2 DBU, E 56602-33-6 BOP reagent, F 101-84-8 PhOPh

SOL 75-05-8 MeCN

CON 5 - 10 minutes, room temperature

STAGE(2)

RCT AS 108-95-2

CON 10 hours, room temperature

PRO AT 16347-97-0

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 35 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 145:47552 CASREACT

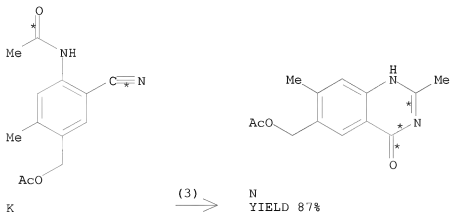
TITLE: Chemical Development of ZD9331: Synthesis of a Bromomethylquinazolinone Avoiding a Nonselective Radical Bromination

AUTHOR(S): Bentley, Dagmar; Godfrey, Andrew A.; Warren, Kenneth E. H.

CORPORATE SOURCE: Process Research and Development Department, AstraZeneca, Macclesfield, Cheshire, SK10 2NA, UK

SOURCE: Organic Process Research & Development (2006), 10(3), 553-555
 CODEN: OPRDFK; ISSN: 1083-6160
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB An efficient regiospecific synthesis of ZD9331 Pivaloyloxymethyl (POM) Bromide has been accomplished via ZD9331 Quinacetate HCl avoiding a nonselective bromination. The original route used a radical bromination on a substrate with three Me groups, which generated a range of bromomethyl derived compds. that carried through to the final active pharmaceutical ingredient (API). A strategy, based on the Zinin reaction, was developed to synthesize the required bromomethyl compound in a regioselective manner. This approach was successfully scaled to manufacture a ton of material.

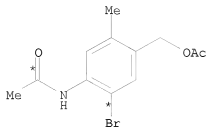
RX(3) OF 6 ...K ==> N



RX(3) RCT K 838858-87-0
 RGT O 7647-01-0 HCl
 PRO N 838858-86-9
 SOL 57-55-6 MeCHOHCH2OH
 CON SUBSTAGE(1) 60 minutes, room temperature
 SUBSTAGE(2) 30 deg C
 NTE HCl gas used

RX(5) OF 6 COMPOSED OF RX(2), RX(3)

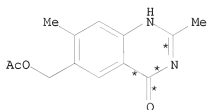
RX(5) B + D ==> N



B



D



N

YIELD 87%

RX(2) RCT B 838858-88-1, D 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT L 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

SUBSTAGE(3) 90 deg C -> 50 deg C

PRO K 838858-87-0

RX(3)

RCT K 838858-87-0

RGT O 7647-01-0 HCl

PRO N 838858-86-9

SOL 57-55-6 MeCHOHCH2OH

CON SUBSTAGE(1) 60 minutes, room temperature

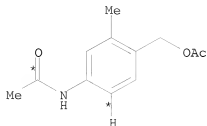
SUBSTAGE(2) 30 deg C

NTE HCl gas used

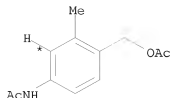
RX(6) OF 6 COMPOSED OF RX(1), RX(2), RX(3)

RX(6) 2 A + D ==> N

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A

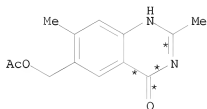


A



D

3
STEPS
→



N
YIELD 87%

RX(1)

STAGE(1)

RGT D 544-92-3 CuCN, E 121-44-8 Et3N, F 75-36-5 AcCl

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 30 minutes, 50 deg C

SUBSTAGE(5) 50 deg C -> 20 deg C

STAGE(2)

RCT A 890086-36-9

RGT G 77-48-5 Br2-Me2-hydantoin

SOL 75-05-8 MeCN

CON SUBSTAGE(1) 60 minutes, 50 deg C

SUBSTAGE(2) 50 deg C -> 20 deg C

STAGE(3)

RGT H 7732-18-5 Water

PRO B 838858-88-1, C 890086-37-0

NTE regioselective

RX(2) RCT B 838858-88-1, D 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT L 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

SUBSTAGE(3) 90 deg C -> 50 deg C

PRO K 838858-87-0

RX(3)

RCT K 838858-87-0

RGT O 7647-01-0 HCl

PRO N 838858-86-9

SOL 57-55-6 MeCHOHCH2OH

CON SUBSTAGE(1) 60 minutes, room temperature

SUBSTAGE(2) 30 deg C

NTE HCl gas used

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 36 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:432671 CASREACT

TITLE: Synthesis and structure of
4-amino-1,2-dihydro-2-oxo-3-quinolinecarboxylate
esters

AUTHOR(S): Ukrainets, I. V.; Bezugly, P. O.; Nicola, Skaif;
Gorokhova, O. V.; Sidorenko, L. V.

CORPORATE SOURCE: Nats. Farm. Univ., Kharkov, 61002, Ukraine

SOURCE: Zhurnal Organichnoi ta Farmatsevtichnoi Khimii (2004),
2(2), 56-61

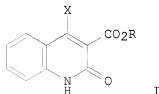
CODEN: ZOFKAM

PUBLISHER: Natsional'nii Farmatsevtichnii Universitet

DOCUMENT TYPE: Journal

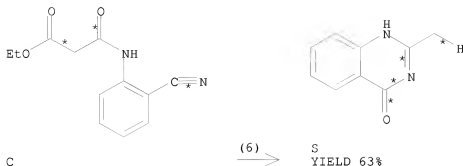
LANGUAGE: Russian

GI



AB Title compds. I (R = Me, Et; X = NH₂) were prepared by heterocyclization of 2-NCC6H₄NHCOCH₂COOEt in R₂Na/ROH. I (R = Et, X = NH₂) was also prepared from I (R = Et, X = Cl) via a pyridinium salt. I (R = Me, X = NH₂) was subjected to x-ray anal.

RX(6) OF 26 ...C ==> S



RX(6) RCT C 130427-06-4

STAGE(1)

RGT R 1310-58-3 KOH
 SOL 7732-18-5 Water
 CON 5 hours, reflux

STAGE(2)

RGT G 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON pH 4

PRO S 1769-24-0

NTE alternative preparation shown, product depends on temperature

L3 ANSWER 37 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:370022 CASREACT

TITLE: Studies on quinazolines, 12. Design of
 4-amino-8-arylquinazoline derivatives as potential
 non-peptide corticotropin-releasing hormone receptor 1
 (CRHR1) antagonists

AUTHOR(S): Wu, Fe-lin Lin; Chen, Grace Shiahuy; Chen, Mei-Yu;
 Cheng, Fong-Chi; Chern, Ji-Wang
 CORPORATE SOURCE: School of Pharmacy, College of Medicine, National
 Taiwan University, Taichung, Taiwan

SOURCE: Chinese Pharmaceutical Journal (Taipei, Taiwan)
 (2004), 56(2), 97-109

CODEN: CPHJEP; ISSN: 1016-1015

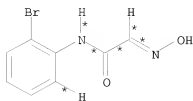
PUBLISHER: Pharmaceutical Society of Republic of China

DOCUMENT TYPE: Journal

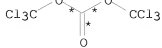
LANGUAGE: English

AB Four 8-aryl-4-(N-cyclopropylmethyl-N-propyl)amino-2-methylquinazolines
 were synthesized, and their binding affinity for corticotropin-releasing
 hormone type 1 receptor (CRHR1) was investigated. Two of the compds.
 possessed high rCRHR1 affinities of $K_i = 13$ and 50 nM. The quinazoline
 derivs. showed comparable SAR to the other known bicyclic system; the
 ortho-substituent on the 8-aryl ring is indispensable.

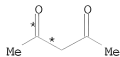
RX(52) OF 92 COMPOSED OF RX(2), RX(3), RX(4), RX(5), RX(6)
 RX(52) C + L + R ==> S



C

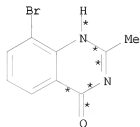


L



R

5
 STEPS
 →



S

YIELD 51%

RX(2) RCT C 101080-38-0
 RGT E 7664-93-9 H2SO4
 PRO H 20780-74-9
 CON 30 minutes, 85 - 87 deg C

RX(3) RCT H 20780-74-9

STAGE(1)

RGT J 1310-73-2 NaOH, K 7722-84-1 H2O2
 SOL 7732-18-5 Water
 CON 0 deg C

STAGE(2)

RGT D 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON pH 4

PRO I 20776-51-6

RX(4) RCT I 20776-51-6, L 32315-10-9
 PRO M 331646-98-1
 SOL 109-99-9 THF
 CON 2 hours, reflux

RX(5) RCT M 331646-98-1
 RGT P 1336-21-6 NH4OH, Q 631-61-8 NH4OAc
 PRO O 437998-34-0
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) 60 deg C -> 95 deg C

SUBSTAGE(2) 1 hour, 95 deg C

RX(6) RCT O 437998-34-0, R 123-54-6
 PRO S 221298-74-4
 CAT 104-15-4 TsOH
 SOL 75-05-8 MeCN
 CON 3 hours, reflux
 NTE alternative solvent/THF shown

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 38 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:292686 CASREACT

TITLE: Multi-component synthesis of 3,2-substituted
 quinazolin-4(3H)-ones under solvent-free conditions

AUTHOR(S): Dandia, Anshu; Singh, Ruby; Sarawgi, Pritima

CORPORATE SOURCE: Department of Chemistry, University of Rajasthan,
 Jaipur, 302004, India

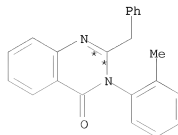
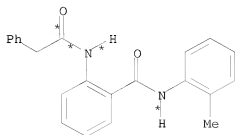
SOURCE: International Electronic Conferences on Synthetic
 Organic Chemistry, 5th, 6th, Sept. 1-30, 2001 and 2002
 [and] 7th, 8th, Nov. 1-30, 2003 and 2004 (2004),
 1116-1122. Editor(s): Seijas, Julio A. Molecular
 Diversity Preservation International: Basel, Switz.
 CODEN: 69GTCO

DOCUMENT TYPE: Conference; (computer optical disk)

LANGUAGE: English

AB Rapid one-pot solvent-free procedure has been developed for the synthesis
 of 2,3-disubstituted quinazolin-4(3H)-ones by neat three component
 cyclocondensation of anthranilic acid, Ph acetyl chloride/benzoyl chloride
 and substituted anilines under microwave irradiation. The exptl. methodol. and
 microwave conditions described here are well established, allowing
 significant rate enhancement and good yields compared to multistep
 conventional reaction conditions. The reaction is generalized for o, m &
 p substituted anilines with electron donating and withdrawing groups to
 give quinazolin-4(3H)-ones. Ortho substituted anilines fail to undergo
 ring closure quinazolines under conventional conditions. The detailed
 reaction mechanism of title reaction has also been discussed.

RX(2) OF 22 ...E ==> D



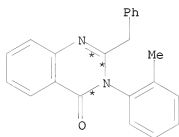
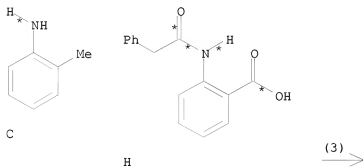
E

D

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RX(2) RCT E 879126-67-7
PRO D 19857-39-7
CAT 104-15-4 TsOH
SOL 68-12-2 DMF
NTE microwave irradiatn., alternative preparation shown

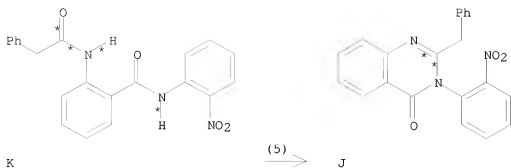
RX(3) OF 22 C + H ==> D



D
YIELD 91%

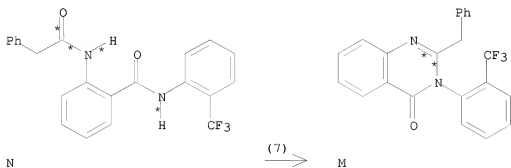
RX(3) RCT C 95-53-4, H 28565-98-2
PRO D 19857-39-7
CON 4 minutes
NTE microwave irradiatn., 640 W used, alternative preparation shown

RX(5) OF 22 ...K ==> J



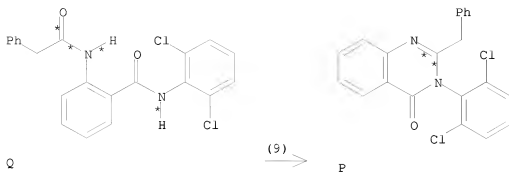
RX(5) RCT K 879126-68-8
 PRO J 201293-03-0
 CAT 104-15-4 TsOH
 SOL 68-12-2 DMF
 NTE microwave irradiation, alternative preparation shown

RX(7) OF 22 ...N ==> M



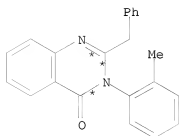
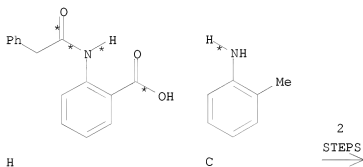
RX(7) RCT N 848085-17-6
 PRO M 848085-22-3
 CAT 104-15-4 TsOH
 SOL 68-12-2 DMF
 NTE microwave irradiation, alternative preparation shown

RX(9) OF 22 ...Q ==> P



RX(9) RCT Q 824972-68-1
 PRO P 381194-40-7
 CAT 104-15-4 TsOH
 SOL 68-12-2 DMF
 NTE microwave irradiat., alternative preparation shown

RX(19) OF 22 COMPOSED OF RX(15), RX(2)
 RX(19) H + C ==> D



RX(15) RCT H 28565-98-2
 STAGE(1)

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RGT AB 1318-93-0 Montmorillonite, AC 108-24-7 Ac2O

STAGE(2)

RCT C 95-53-4

PRO E 879126-67-7

NTE chemoselective, green chem., microwave irradi., Montmorillonite
KSF used

RX(2) RCT E 879126-67-7

PRO D 19857-39-7

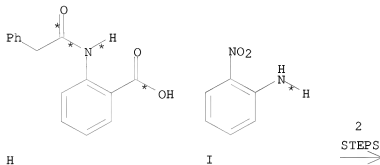
CAT 104-15-4 TsOH

SOL 68-12-2 DMF

NTE microwave irradi., alternative preparation shown

RX(20) OF 22 COMPOSED OF RX(16), RX(5)

RX(20) H + I ==> J



J

RX(16) RCT H 28565-98-2

STAGE(1)

RGT AB 1318-93-0 Montmorillonite, AC 108-24-7 Ac2O

STAGE(2)

RCT I 88-74-4

PRO K 879126-68-8

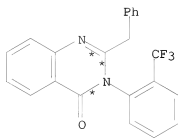
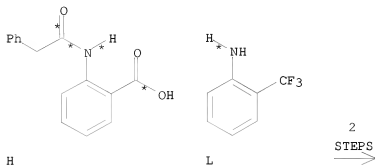
NTE chemoselective, green chem., microwave irradi., Montmorillonite

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KSF used

RX(5) RCT K 879126-68-8
PRO J 201293-03-0
CAT 104-15-4 TsOH
SOL 68-12-2 DMF
NTE microwave irradsn., alternative preparation shown

RX(21) OF 22 COMPOSED OF RX(17), RX(7)
RX(21) H + L ==> M



M

RX(17) RCT H 28565-98-2

STAGE(1)

RGT AB 1318-93-0 Montmorillonite, AC 108-24-7 Ac2O

STAGE(2)

RCT L 88-17-5

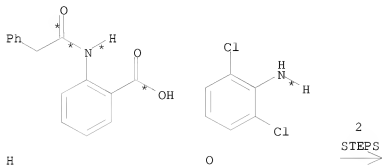
PRO N 848085-17-6

NTE chemoselective, green chem., microwave irradsn., Montmorillonite
KSF used

RX(7) RCT N 848085-17-6
PRO M 848085-22-3
CAT 104-15-4 TsOH
SOL 68-12-2 DMF
NTE microwave irradsn., alternative preparation shown

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RX(22) OF 22 COMPOSED OF RX(18), RX(9)
 RX(22) H + O ==> P



P

RX(18) RCT H 28565-98-2

STAGE(1)

RGT AB 1318-93-0 Montmorillonite, AC 108-24-7 Ac2O

STAGE(2)

RCT O 608-31-1

PRO Q 824972-68-1

NTE chemoselective, green chem., microwave irradiation, Montmorillonite KSF used

RX(9)

RCT Q 824972-68-1

PRO P 381194-40-7

CAT 104-15-4 TsOH

SOL 68-12-2 DMF

NTE microwave irradiation, alternative preparation shown

REFERENCE COUNT:

29

THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 39 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:205151 CASREACT

TITLE: Discovery of potent and selective PARP-1 and PARP-2 inhibitors: SBDD analysis via a combination of X-ray structural study and homology modeling

AUTHOR(S): Ishida, Junya; Yamamoto, Hirofumi; Kido, Yoshiyuki; Kamiyo, Kazunori; Murano, Kenji; Miyake, Hiroshi; Ohkubo, Mitsuru; Kinoshita, Takayoshi; Warizaya, Masaichi; Iwashita, Akinori; Mihara, Kayoko; Matsuoka, Nobuya; Hattori, Kouji

CORPORATE SOURCE: Medicinal Chemistry Research Laboratories, Fujisawa Pharmaceutical Co. Ltd, 5-2-3 Tokodai, Tsukuba, Ibaraki, 300-2698, Japan

SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(5), 1378-1390

CODEN: BMECEP; ISSN: 0968-0896

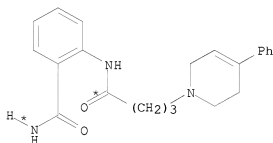
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We disclose herein our efforts aimed at discovery of selective PARP-1 and PARP-2 inhibitors. We have recently discovered several novel classes of quinazolinones, quinazolidinones, and quinoxalines as potent PARP-1 inhibitors, which may represent attractive therapeutic candidates. In PARP enzyme assays using recombinant PARP-1 and PARP-2, the quinazolinone derivs. displayed relatively high selectivity for PARP-1 and quinoxaline derivs. showed superior selectivity for PARP-2, and the quinazolidinone derivs. did not have selectivity for PARP-1/2. Structure-based drug design anal. via a combination of X-ray structural study utilizing the complexes of inhibitors and human PARP-1 catalytic domain, and homol. modeling using murine PARP-2 suggested distinct interactions of inhibitors with PARP-1 and PARP-2. These findings provide a new structural framework for the design of selective inhibitors for PARP-1 and PARP-2.

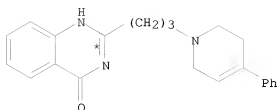
RX(2) OF 47 ...P ==> D



P

(2) →

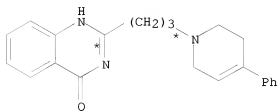
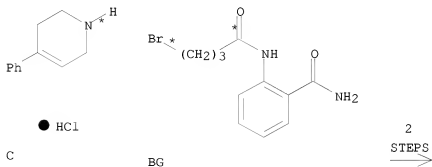
10/ 562,112



D
YIELD 74%

RX(2) RCT P 437998-41-9
RGT J 1310-73-2 NaOH
PRO D 437995-37-4
SOL 7732-18-5 Water, 123-91-1 Dioxane
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 15 hours, room temperature

RX(35) OF 47 COMPOSED OF RX(26), RX(2)
RX(35) C + BG ==> D



D
YIELD 74%

RX(26) RCT C 43064-12-6, BG 437998-35-1
STAGE(1)
RGT T 121-44-8 Et3N

SOL 68-12-2 DMF
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> room temperature
 SUBSTAGE(3) 24 hours, room temperature

STAGE(2)
 RGT N 7732-18-5 Water
 CON room temperature

PRO P 437998-41-9

RX(2) RCT P 437998-41-9
 RGT J 1310-73-2 NaOH
 PRO D 437995-37-4
 SOL 7732-18-5 Water, 123-91-1 Dioxane
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 15 hours, room temperature

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 40 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:192275 CASREACT

TITLE: Preparation of quinazolinone derivatives useful for the regulation of glucose homeostasis and food intake

INVENTOR(S): Rudolph, Joachim; O'Connor, Stephen; Coish, Philip; Wickens, Philip; Bondar, Georgiy; Chuang, Chih-Yuan; Ramsden, Philip; Lowe, Derek; Bierer, Donald; Chen, Libing; Fu, Wenlang; Khire, Uday; Liu, Xiao-Gao; McClure, Andrea; Wang, Lei; Yi, Lin; Esler, William

PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA

SOURCE: PCT Int. Appl., 559 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

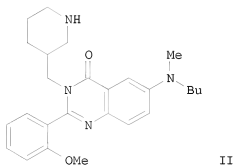
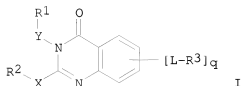
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006012577	A2	20060202	WO 2005-US26192	20050722
WO 2006012577	A3	20060928		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.: US 2004-590804P 20040722

OTHER SOURCE(S): MARPAT 144:192275

GI

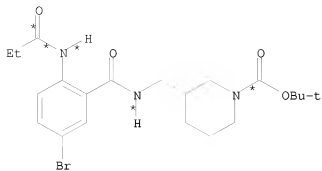


AB The invention is related to substituted quinazolinone derivs. I [R1 = (un)substituted pyrrolidin-3-yl, piperidin-3-yl, morpholin-4-yl, etc.; R2 = H, (un)substituted cyclo/alkyl, pyridinyl, Ph, etc.; R3 = H, halo, haloalkyl, (un)substituted Ph, alkyl, etc.; L = a bond, O, CO, S, SO2, NHSO2, NH and derivs., etc.; X = (CH2)m; m = 0-2; Y = (CH2)n; n = 1-2; p = 0-2; with provisos], and their pharmaceutically acceptable salts, and their comps., and methods for treating diabetes, obesity and related disorders, and regulation of glucose homeostasis and food intake (e.g., stimulation and suppression) (no data). The invention is also related to the preparation of quinazolinones I. Five biol. tests are given (no data). Thus, II•TFA was prepared by amination of 5-fluoro-2-nitrobenzoic acid with N-methylbutylamine, reduction of the nitro compound, cyclocondensation with

o-anisoyl chloride, reaction with tert-Bu
3-(aminomethyl)piperidine-1-carboxylate (intermediate not isolated), and
Boc-deprotection in the presence of TFA.

RX(128) OF 652 KL + Z ==> BH...

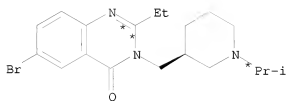
10/ 562,112



KL



(128)



BH

RX(128) RCT KL 875269-77-5

STAGE(1)

SOL 64-19-7 AcOH

CON 2 hours, 100 deg C

STAGE(2)

RCT Z 75-30-9

RGT AB 584-08-7 K2CO3

SOL 75-05-8 MeCN

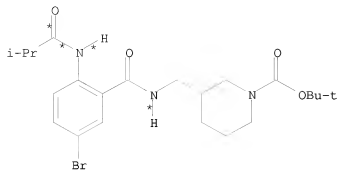
CON 4 hours, 70 deg C

PRO BH 875269-76-4

NTE sealed vial used in stage 1

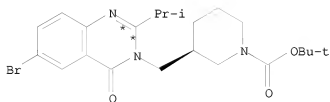
RX(137) OF 652 ...KT ==> KS...

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KT

(137)
→

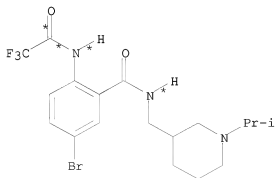


KS

YIELD 38%

RX(137) RCT KT 875269-98-0
RGT EB 1310-65-2 LiOH
PRO KS 875269-86-6
SOL 107-21-1 (CH2OH)2
CON 15 hours, 130 deg C

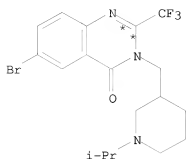
RX(162) OF 652 ...LQ ==> FL...



LQ

(162)
→

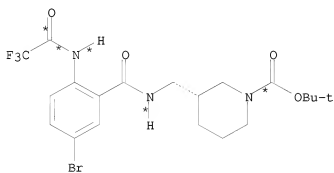
10/ 562,112



FL
YIELD 95%

RX(162) RCT LQ 875270-14-7
PRO FL 875270-15-8
CON 1 hour, 200 deg C
NTE thermal, sealed vial used

RX(164) OF 652 ...LR + C ==> LS...



LR

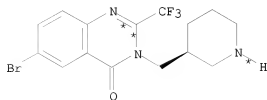


C

(164) \longrightarrow



LS: CM 1
YIELD 100%



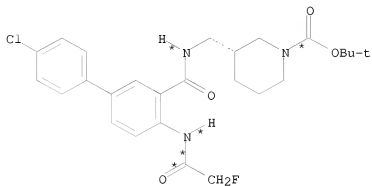
LS: CM 2
YIELD 100%

RX(164) RCT LR 875270-16-9, C 76-05-1
PRO LS 875270-18-1

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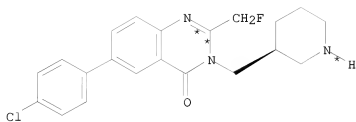
CON 1 hour, 150 deg C
NTE microwave irradiation

RX(169) OF 652 ...LX ==> GC...



LX

(169)
→

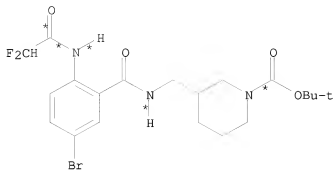


GC
YIELD 87%

RX(169) RCT LX 875270-26-1
RGT LY 109-63-7 BF3-Et2O
PRO GC 875270-27-2
SOL 64-19-7 AcOH
CON 25 minutes, 130 deg C
NTE microwave irradiation

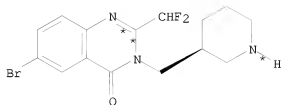
RX(171) OF 652 ...MA ==> MD...

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MA

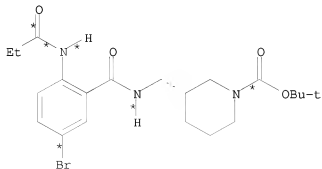
(171)



MD

RX(171) RCT MA 875270-28-3
 PRO MD 875270-29-4
 SOL 64-19-7 AcOH
 CON 2 hours, 100 deg C
 NTE sealed vial used

RX(264) OF 652 COMPOSED OF RX(128), RX(19)
 RX(264) KL + Z + AZ ==> BI

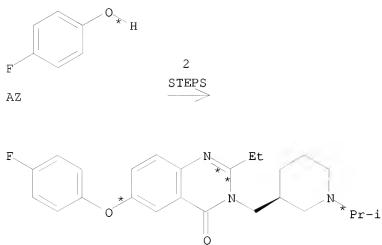


KL



Z

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BI

RX(128) RCT KL 875269-77-5

STAGE(1)

SOL 64-19-7 AcOH

CON 2 hours, 100 deg C

STAGE(2)

RCT Z 75-30-9

RGT AB 584-08-7 K₂CO₃

SOL 75-05-8 MeCN

CON 4 hours, 70 deg C

PRO BH 875269-76-4

NTE sealed vial used in stage 1

RX(19) RCT AZ 371-41-5, BH 875269-76-4

RGT BC 1118-71-4 3,5-Heptanedione, 2,2,6,6-tetramethyl-, AH 534-17-8
Cs₂CO₃

PRO BI 875258-87-0

CAT 7758-89-6 CuCl

SOL 872-50-4 NMEP

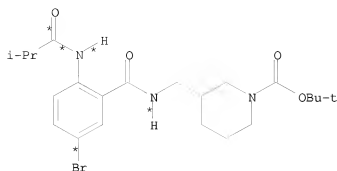
CON 20 minutes, room temperature -> 205 deg C

NTE thermal, microwave irradiation, sealed tube used, Ullmann
coupling reaction

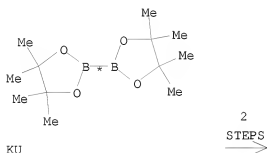
RX(285) OF 652 COMPOSED OF RX(137), RX(138)

RX(285) KT + KU ==> KV

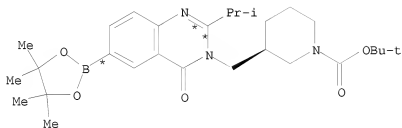
10/ 562,112



KT



KU



KV

YIELD 82%

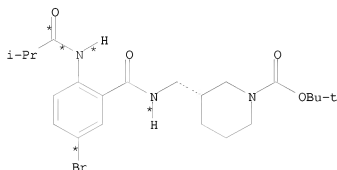
RX(137) RCT KT 875269-98-0
RGT EB 1310-65-2 LiOH
PRO KS 875269-86-6
SOL 107-21-1 (CH₂OH)₂
CON 15 hours, 130 deg C

RX(138) RCT KS 875269-86-6, KU 73183-34-3
RGT KW 127-08-2 AcOK
PRO KV 875269-87-7
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-
SOL 68-12-2 DMF

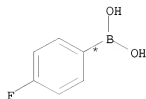
10/ 562,112

CON SUBSTAGE(1) 2 minutes, room temperature
 SUBSTAGE(2) 15 hours, room temperature -> 60 deg C
 SUBSTAGE(3) 60 deg C -> room temperature
 NTE Suzuki coupling reaction

RX(286) OF 652 COMPOSED OF RX(137), RX(151)
 RX(286) KT + GE ==> DT

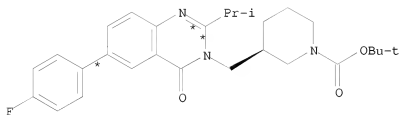


KT



GE

2
 STEPS
 →



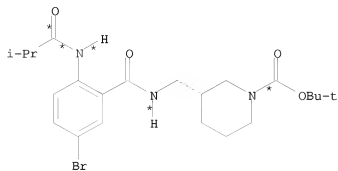
DT
 YIELD 94%

RX(137) RCT KT 875269-98-0
 RGT EB 1310-65-2 LiOH
 PRO KS 875269-86-6
 SOL 107-21-1 (CH2OH)2
 CON 15 hours, 130 deg C

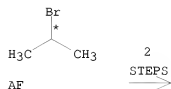
RX(151) RCT KS 875269-86-6, GE 1765-93-1
 RGT AB 584-08-7 K2CO3
 PRO DT 875269-99-1
 CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-
 κP)ferrocene]dichloro-, (SP-4-2)-
 SOL 7732-18-5 Water, 123-91-1 Dioxane, 108-88-3 PhMe
 CON 15 hours, 80 deg C
 NTE Suzuki coupling reaction

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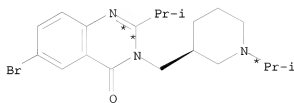
RX(287) OF 652 COMPOSED OF RX(137), RX(157)
RX(287) KT + AF ==> ET



KT



2
STEPS
→



ET

RX(137) RCT KT 875269-98-0
RGT EB 1310-65-2 LiOH
PRO KS 875269-86-6
SOL 107-21-1 (CH₂OH)₂
CON 15 hours, 130 deg C

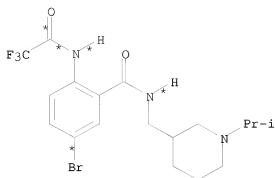
RX(157) RCT KS 875269-86-6

STAGE(1)
RGT C 76-05-1 F₃CCO₂H
SOL 75-09-2 CH₂Cl₂
CON 3 hours, room temperature

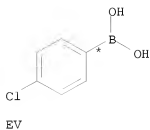
STAGE(2)
RCT AF 75-26-3
RGT AH 534-17-8 Cs₂CO₃
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 14 hours, 70 deg C
SUBSTAGE(2) 70 deg C -> room temperature

PRO ET 875270-09-0

RX(318) OF 652 COMPOSED OF RX(162), RX(57)
RX(318) LQ + EV ==> FM

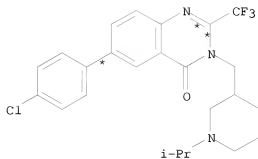


LQ



EV

2
STEPS
→



FM

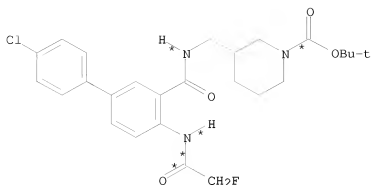
YIELD 14%

RX(162) RCT LQ 875270-14-7
 PRO FL 875270-15-8
 CON 1 hour, 200 deg C
 NTE thermal, sealed vial used

RX(57) RCT EV 1679-18-1, FL 875270-15-8
 RGT AB 584-08-7 K2CO3
 PRO FM 875259-36-2
 CAT 95464-05-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-, compd. with dichloromethane (1:1)
 SOL 109-99-9 THF
 CON 20 minutes, room temperature -> 150 deg C
 NTE thermal, microwave irradiation, Suzuki coupling reaction, sealed tube used

RX(320) OF 652 COMPOSED OF RX(164), RX(165)
 RX(320) LR + C + Z ==> FN

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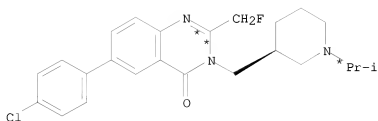


LX



Z

2
STEPS
→



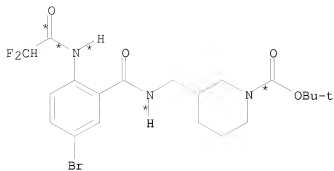
GD
YIELD 27%

RX(169) RCT LX 875270-26-1
RGT LY 109-63-7 BF3-Et2O
PRO GC 875270-27-2
SOL 64-19-7 AcOH
CON 25 minutes, 130 deg C
NTE microwave irradiation

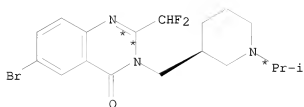
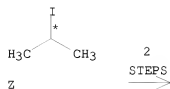
RX(66) RCT Z 75-30-9, GC 875270-27-2
RGT AH 534-17-8 Cs2CO3
PRO GD 875259-45-3
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 15 hours, room temperature -> 70 deg C
SUBSTAGE(2) 70 deg C -> room temperature

RX(327) OF 652 COMPOSED OF RX(171), RX(172)
RX(327) MA + Z ==> GF

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MA



GF

YIELD 81%

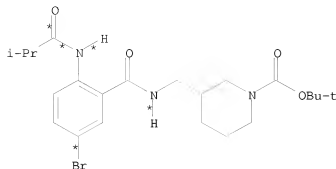
RX(171) RCT MA 875270-28-3
PRO MD 875270-29-4
SOL 64-19-7 AcOH
CON 2 hours, 100 deg C
NTE sealed vial used

RX(172) RCT Z 75-30-9, MD 875270-29-4
RGT AB 584-08-7 K2CO3
PRO GF 875270-30-7
SOL 75-05-8 MeCN
CON 4 hours, 70 deg C

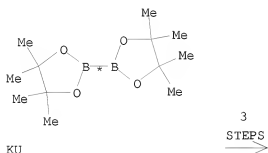
RX(461) OF 652 COMPOSED OF RX(137), RX(138), RX(139)

RX(461) KT + KU ==> KX

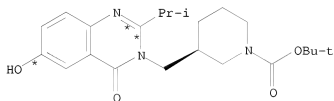
10/ 562,112



KT



KU



KX

YIELD 88%

RX(137) RCT KT 875269-98-0
RGT EB 1310-65-2 LiOH
PRO KS 875269-86-6
SOL 107-21-1 (CH2OH)2
CON 15 hours, 130 deg C

RX(138) RCT KS 875269-86-6, KU 73183-34-3
RGT KW 127-08-2 AcOK
PRO KV 875269-87-7
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino- κ P)ferrocene]dichloro-, (SP-4-2)-
SOL 68-12-2 DMF
CON SUBSTAGE(1) 2 minutes, room temperature
SUBSTAGE(2) 15 hours, room temperature -> 60 deg C

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SUBSTAGE(3) 60 deg C -> room temperature
NTE Suzuki coupling reaction

RX(139) RCT KV 875269-87-7

STAGE(1)

RGT E 1310-73-2 NaOH, KY 7722-84-1 H2O2

SOL 7732-18-5 Water, 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RGT CC 12125-02-9 NH4Cl

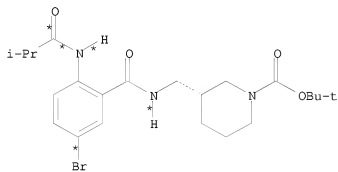
SOL 7732-18-5 Water

CON pH 7.0

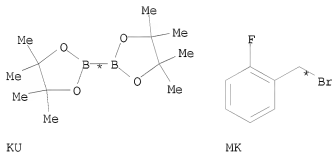
PRO KX 875269-88-8

RX(462) OF 652 COMPOSED OF RX(137), RX(138), RX(178)

RX(462) KT + KU + MK ==> ML

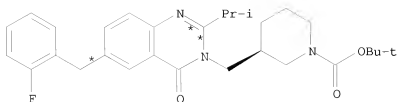


KT



KU

MK



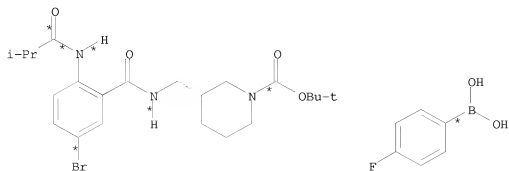
ML
YIELD 71%

RX(137) RCT KT 875269-98-0
RGT EB 1310-65-2 LiOH
PRO KS 875269-86-6
SOL 107-21-1 (CH₂OH)₂
CON 15 hours, 130 deg C

RX(138) RCT KS 875269-86-6, KU 73183-34-3
RGT KW 127-08-2 AcOK
PRO KV 875269-87-7
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-
SOL 68-12-2 DMF
CON SUBSTAGE(1) 2 minutes, room temperature
SUBSTAGE(2) 15 hours, room temperature -> 60 deg C
SUBSTAGE(3) 60 deg C -> room temperature
NTE Suzuki coupling reaction

RX(178) RCT KV 875269-87-7, MK 446-48-0
RGT AB 584-08-7 K₂CO₃
PRO ML 875270-37-4
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-
SOL 123-91-1 Dioxane, 108-88-3 PhMe
CON SUBSTAGE(1) 1 minute
SUBSTAGE(2) 15 hours, 90 deg C
SUBSTAGE(3) 90 deg C -> room temperature

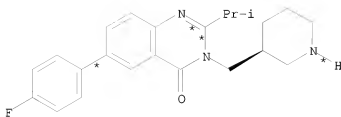
RX(463) OF 652 COMPOSED OF RX(137), RX(151), RX(42)
RX(463) KT + GE ==> DU



KT

GE

3
STEPS
→



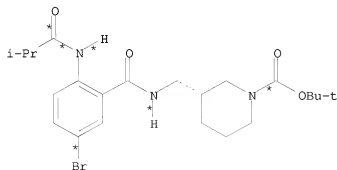
DU
YIELD 96%

RX(137) RCT KT 875269-98-0
RGT EB 1310-65-2 LiOH
PRO KS 875269-86-6
SOL 107-21-1 (CH2OH)2
CON 15 hours, 130 deg C

RX(151) RCT KS 875269-86-6, GE 1765-93-1
RGT AB 584-08-7 K2CO3
PRO DT 875269-99-1
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-
SOL 7732-18-5 Water, 123-91-1 Dioxane, 108-88-3 PhMe
CON 15 hours, 80 deg C
NTE Suzuki coupling reaction

RX(42) RCT DT 875269-99-1
RGT C 76-05-1 F3CCO2H
PRO DU 875259-16-8
SOL 75-09-2 CH2Cl2
CON 15 hours, room temperature

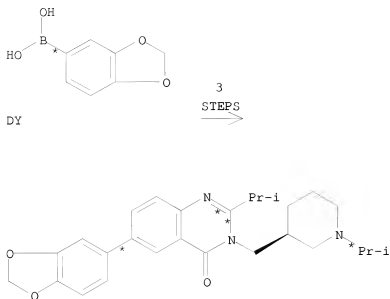
RX(464) OF 652 COMPOSED OF RX(137), RX(157), RX(50)
RX(464) KT + AF + DY ==> EU



KT

AF

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EU
YIELD 56%

RX(137) RCT KT 875269-98-0
RGT EB 1310-65-2 LiOH
PRO KS 875269-86-6
SOL 107-21-1 (CH2OH)2
CON 15 hours, 130 deg C

RX(157) RCT KS 875269-86-6

STAGE(1)
RGT C 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2
CON 3 hours, room temperature

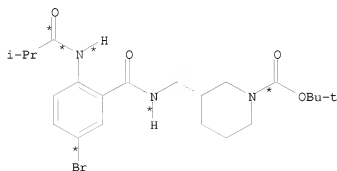
STAGE(2)
RCT AF 75-26-3
RGT AH 534-17-8 Cs2CO3
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 14 hours, 70 deg C
SUBSTAGE(2) 70 deg C -> room temperature

PRO ET 875270-09-0

RX(50) RCT DY 94839-07-3, ET 875270-09-0
RGT AB 584-08-7 K2CO3
PRO EU 875259-29-3
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-
7732-18-5 Water, 127-19-5 AcNMe2
CON SUBSTAGE(1) 15 minutes, 130 deg C
SUBSTAGE(2) 130 deg C -> room temperature
NTE microwave irradiation, Suzuki coupling reaction, sealed vial used

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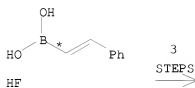
RX(465) OF 652 COMPOSED OF RX(137), RX(157), RX(77)
 RX(465) KT + AF + HF ==> HG



KT

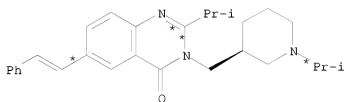


AF



HF

3
STEPS
→



HG

RX(137) RCT KT 875269-98-0
 RGT EB 1310-65-2 LiOH
 PRO KS 875269-86-6
 SOL 107-21-1 (CH2OH)2
 CON 15 hours, 130 deg C

RX(157) RCT KS 875269-86-6

STAGE(1)

RGT C 76-05-1 F3CCO2H
 SOL 75-09-2 CH2Cl2
 CON 3 hours, room temperature

STAGE(2)

RCT AF 75-26-3

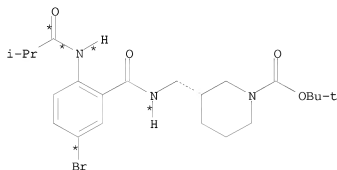
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RGT AH 534-17-8 Cs2CO3
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 14 hours, 70 deg C
SUBSTAGE(2) 70 deg C -> room temperature

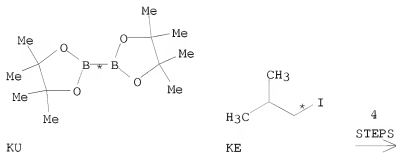
PRO ET 875270-09-0

RX(77) RCT ET 875270-09-0, HF 6783-05-7
RGT AB 584-08-7 K2CO3
PRO HG 875259-62-4
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-
κP)ferrocene]dichloro-, (SP-4-2)-
SOL 7732-18-5 Water, 127-19-5 AcNMe2
CON SUBSTAGE(1) 15 minutes, 130 deg C
SUBSTAGE(2) 130 deg C -> room temperature
NTE stereoselective, microwave irradiation, sealed tube used, Suzuki
coupling reaction

RX(480) OF 652 COMPOSED OF RX(137), RX(138), RX(139), RX(140)
RX(480) KT + KU + KE ==> KZ

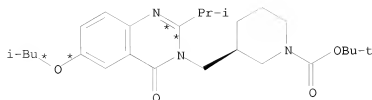


KT



KU

KE



KZ
YIELD 74%

RX(137) RCT KT 875269-98-0
RGT EB 1310-65-2 LiOH
PRO KS 875269-86-6
SOL 107-21-1 (CH2OH)2
CON 15 hours, 130 deg C

RX(138) RCT KS 875269-86-6, KU 73183-34-3
RGT KW 127-08-2 AcOK
PRO KV 875269-87-7
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-
SOL 68-12-2 DMF
CON SUBSTAGE(1) 2 minutes, room temperature
SUBSTAGE(2) 15 hours, room temperature -> 60 deg C
SUBSTAGE(3) 60 deg C -> room temperature
NTE Suzuki coupling reaction

RX(139) RCT KV 875269-87-7

STAGE(1)
RGT E 1310-73-2 NaOH, KY 7722-84-1 H2O2
SOL 7732-18-5 Water, 109-99-9 THF
CON 1 hour, room temperature

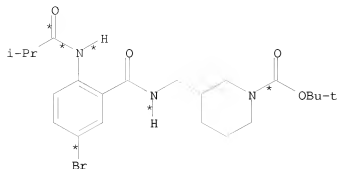
STAGE(2)
RGT CC 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON pH 7.0

PRO KX 875269-88-8

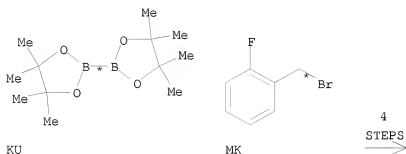
RX(140) RCT KE 513-38-2, KX 875269-88-8
RGT AH 534-17-8 Cs2CO3
PRO KZ 875269-89-9
SOL 68-12-2 DMF
CON 15 hours, 90 deg C

RX(481) OF 652 COMPOSED OF RX(137), RX(138), RX(178), RX(179)
RX(481) KT + KU + MK ==> HK

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KT



HK
YIELD 87%

RX(137) RCT KT 875269-98-0
RGT EB 1310-65-2 LiOH
PRO KS 875269-86-6
SOL 107-21-1 (CH₂OH)₂
CON 15 hours, 130 deg C

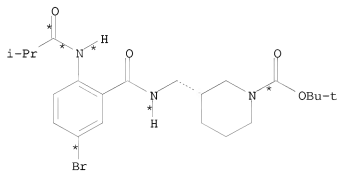
RX(138) RCT KS 875269-86-6, KU 73183-34-3
RGT KW 127-08-2 AcOK
PRO KV 875269-87-7
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-
SOL 68-12-2 DMF
CON SUBSTAGE(1) 2 minutes, room temperature
SUBSTAGE(2) 15 hours, room temperature -> 60 deg C

SUBSTAGE(3) 60 deg C -> room temperature
 NTE Suzuki coupling reaction

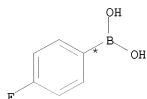
RX(178) RCT KV 875269-87-7, MK 446-48-0
 RGT AB 584-08-7 K2CO3
 PRO ML 875270-37-4
 CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-
 κP)ferrocene]dichloro-, (SP-4-2)-
 SOL 123-91-1 Dioxane, 108-88-3 PhMe
 CON SUBSTAGE(1) 1 minute
 SUBSTAGE(2) 15 hours, 90 deg C
 SUBSTAGE(3) 90 deg C -> room temperature

RX(179) RCT ML 875270-37-4
 RGT C 76-05-1 F3CCO2H
 PRO HK 875270-38-5
 SOL 75-09-2 CH2Cl2
 CON 15 hours, room temperature

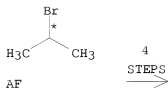
RX(509) OF 652 COMPOSED OF RX(137), RX(151), RX(42), RX(43)
 RX(509) KT + GE + AF ==> DV



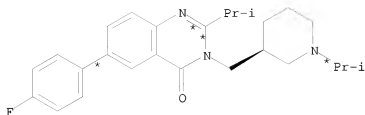
KT



GE



AF



DV

YIELD 77%

RX(137) RCT KT 875269-98-0
 RGT EB 1310-65-2 LiOH
 PRO KS 875269-86-6
 SOL 107-21-1 (CH₂OH)₂
 CON 15 hours, 130 deg C

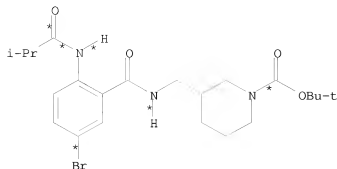
RX(151) RCT KS 875269-86-6, GE 1765-93-1
 RGT AB 584-08-7 K₂CO₃
 PRO DT 875269-99-1
 CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-
 SOL 7732-18-5 Water, 123-91-1 Dioxane, 108-88-3 PhMe
 CON 15 hours, 80 deg C
 NTE Suzuki coupling reaction

RX(42) RCT DT 875269-99-1
 RGT C 76-05-1 F₃CCO₂H
 PRO DU 875259-16-8
 SOL 75-09-2 CH₂Cl₂
 CON 15 hours, room temperature

RX(43) RCT DU 875259-16-8, AF 75-26-3
 RGT AB 584-08-7 K₂CO₃
 PRO DV 875259-17-9
 SOL 75-05-8 MeCN
 CON 4 hours, 70 deg C

RX(515) OF 652 COMPOSED OF RX(137), RX(157), RX(77), RX(78)
 RX(515) KT + AF + HF ==> HH

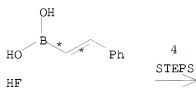
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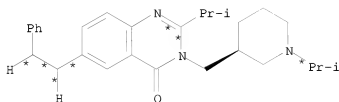
KT



AF



HF



HH

YIELD 90%

RX(137) RCT KT 875269-98-0
RGT EB 1310-65-2 LiOH
PRO KS 875269-86-6
SOL 107-21-1 (CH₂OH)₂
CON 15 hours, 130 deg C

RX(157) RCT KS 875269-86-6

STAGE(1)

RGT C 76-05-1 F₃CCO₂H
SOL 75-09-2 CH₂Cl₂
CON 3 hours, room temperature

STAGE(2)

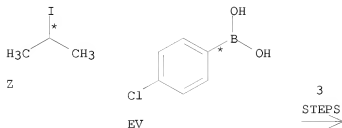
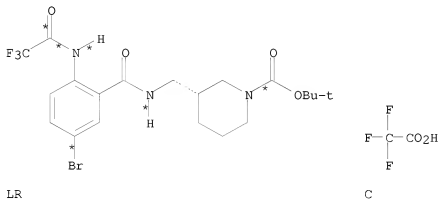
RCT AF 75-26-3
RGT AH 534-17-8 Cs₂CO₃
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 14 hours, 70 deg C
SUBSTAGE(2) 70 deg C -> room temperature

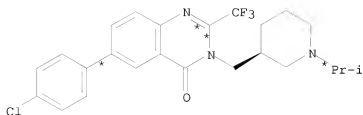
PRO ET 875270-09-0

RX(77) RCT ET 875270-09-0, HF 6783-05-7
 RGT AB 584-08-7 K2CO3
 PRO HG 875259-62-4
 CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-
 κP)ferrocene]dichloro-, (SP-4-2)-
 SOL 7732-18-5 Water, 127-19-5 AcNMe2
 CON SUBSTAGE(1) 15 minutes, 130 deg C
 SUBSTAGE(2) 130 deg C -> room temperature
 NTE stereoselective, microwave irradiation, sealed tube used, Suzuki
 coupling reaction

RX(78) RCT HG 875259-62-4
 RGT HA 1333-74-0 H2
 PRO HH 875259-63-5
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 CON 3 hours, room temperature

RX(526) OF 652 COMPOSED OF RX(164), RX(165), RX(58)
 RX(526) LR + C + Z + EV ==> FO





FO

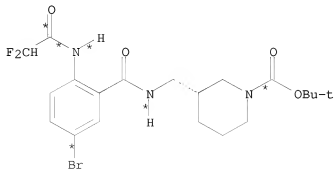
YIELD 86%

RX(164) RCT LR 875270-16-9, C 76-05-1
 PRO LS 875270-18-1
 CON 1 hour, 150 deg C
 NTE microwave irradiation

RX(165) RCT Z 75-30-9, LS 875270-18-1
 RGT AB 584-08-7 K2CO3
 PRO FN 875270-20-5
 SOL 75-05-8 MeCN
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 15 hours, room temperature -> 70 deg C
 SUBSTAGE(3) 70 deg C -> room temperature

RX(58) RCT EV 1679-18-1, FN 875270-20-5
 RGT FC 312959-24-3 Ferrocene,
 1'-[bis(1,1-dimethylethyl)phosphino]-1,2,3,4,5-pentaphenyl-, FD
 13400-13-0 CsF
 PRO FO 875259-37-3
 CAT 52522-40-4 Pd complex
 SOL 109-99-9 THF
 CON 12 hours, room temperature
 NTE Suzuki coupling reaction

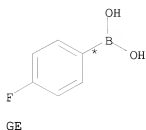
RX(535) OF 652 COMPOSED OF RX(171), RX(172), RX(67)
 RX(535) MA + Z + GE ==> GG



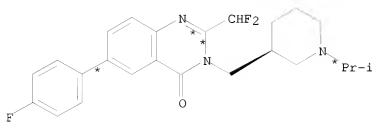
MA



Z



3
STEPS
→



YIELD 42%

RX(171) RCT MA 875270-28-3
PRO MD 875270-29-4
SOL 64-19-7 AcOH
CON 2 hours, 100 deg C
NTE sealed vial used

RX(172) RCT Z 75-30-9, MD 875270-29-4
RGT AB 584-08-7 K2CO3
PRO GF 875270-30-7
SOL 75-05-8 MeCN
CON 4 hours, 70 deg C

RX(67) RCT GE 1765-93-1, GF 875270-30-7

STAGE(1)

RGT FD 13400-13-0 CsF
SOL 109-99-9 THF
CON 20 minutes

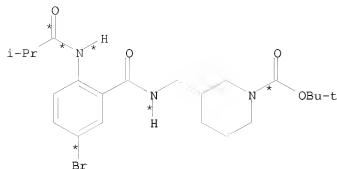
STAGE(2)

RGT FC 312959-24-3 Ferrocene,
1'-[bis(1,1-dimethylethyl)phosphino]-1,2,3,4,5-pentaphenyl-
CAT 52522-40-4 Pd complex
CON 10 hours, room temperature

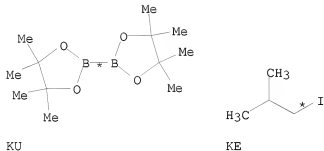
PRO GG 875259-46-4
NTE Suzuki coupling reaction

RX(626) OF 652 COMPOSED OF RX(137), RX(138), RX(139), RX(140), RX(141)
RX(626) KT + KU + KE ==> CS

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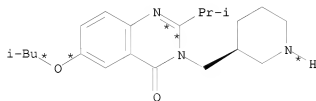


KT



KU

KE



CS

YIELD 79%

RX(137)	RCT	KT 875269-98-0
	RGT	EB 1310-65-2 LiOH
	PRO	KS 875269-86-6
	SOL	107-21-1 (CH ₂ OH) ₂
	CON	15 hours, 130 deg C
RX(138)	RCT	KS 875269-86-6, KU 73183-34-3
	RGT	KW 127-08-2 AcOK
	PRO	KV 875269-87-7
	CAT	72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-
	SOL	68-12-2 DMF
	CON	SUBSTAGE(1) 2 minutes, room temperature

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SUBSTAGE(2) 15 hours, room temperature -> 60 deg C
SUBSTAGE(3) 60 deg C -> room temperature
NTE Suzuki coupling reaction

RX(139) RCT KV 875269-87-7

STAGE(1)

RGT E 1310-73-2 NaOH, KY 7722-84-1 H2O2
SOL 7732-18-5 Water, 109-99-9 THF
CON 1 hour, room temperature

STAGE(2)

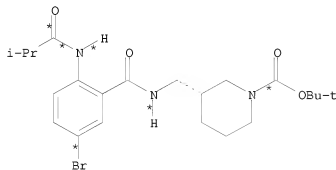
RGT CC 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON pH 7.0

PRO KX 875269-88-8

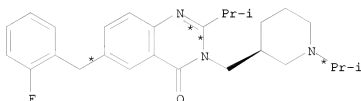
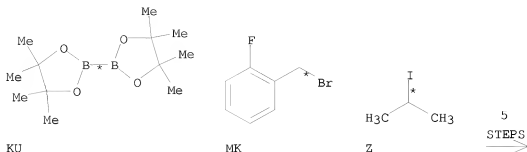
RX(140) RCT KE 513-38-2, KX 875269-88-8
RGT AH 534-17-8 Cs2CO3
PRO KZ 875269-89-9
SOL 68-12-2 DMF
CON 15 hours, 90 deg C

RX(141) RCT KZ 875269-89-9
RGT C 76-05-1 F3CCO2H
PRO CS 875269-90-2
SOL 75-09-2 CH2Cl2
CON 15 hours, room temperature

RX(627) OF 652 COMPOSED OF RX(137), RX(138), RX(178), RX(179), RX(80)
RX(627) KT + KU + MK + Z ==> HL



KT



YIELD 11%

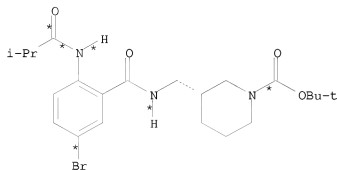
- RX(137) RCT KT 875269-98-0
RGT EB 1310-65-2 LiOH
PRO KS 875269-86-6
SOL 107-21-1 (CH₂OH)₂
CON 15 hours, 130 deg C
- RX(138) RCT KS 875269-86-6, KU 73183-34-3
RGT KW 127-08-2 AcOK
PRO KV 875269-87-7
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-
68-12-2 DMF
SOL SUBSTAGE(1) 2 minutes, room temperature
SUBSTAGE(2) 15 hours, room temperature -> 60 deg C
SUBSTAGE(3) 60 deg C -> room temperature
NTE Suzuki coupling reaction
- RX(178) RCT KV 875269-87-7, MK 446-48-0
RGT AB 584-08-7 K₂CO₃
PRO ML 875270-37-4
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-κP)ferrocene]dichloro-, (SP-4-2)-
SOL 123-91-1 Dioxane, 108-88-3 PhMe
CON SUBSTAGE(1) 1 minute
SUBSTAGE(2) 15 hours, 90 deg C
SUBSTAGE(3) 90 deg C -> room temperature
- RX(179) RCT ML 875270-37-4
RGT C 76-05-1 F₃CCO₂H
PRO HK 875270-38-5
SOL 75-09-2 CH₂Cl₂

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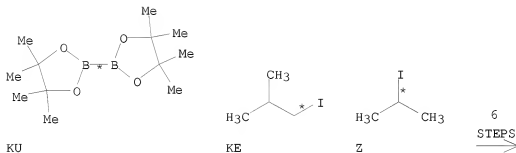
CON 15 hours, room temperature

RX(80) RCT Z 75-30-9, HK 875270-38-5
RGT AH 534-17-8 Cs2CO3
PRO HL 875259-65-7
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 15 hours, room temperature -> 90 deg C
SUBSTAGE(2) 90 deg C -> room temperature

RX(644) OF 652 COMPOSED OF RX(137), RX(138), RX(139), RX(140), RX(141), RX(33)
RX(644) KT + KU + KE + Z ==> CT



KT

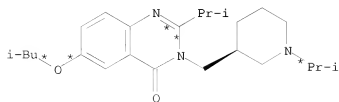


KU

KE

Z

6
STEPS
→



CT
YIELD 30%

RX(137) RCT KT 875269-98-0

RGT EB 1310-65-2 LiOH
PRO KS 875269-86-6
SOL 107-21-1 (CH2OH)2
CON 15 hours, 130 deg C

RX(138) RCT KS 875269-86-6, KU 73183-34-3
RGT KW 127-08-2 AcOK
PRO KV 875269-87-7
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-
κP)ferrocene]dichloro-, (SP-4-2)-
SOL 68-12-2 DMF
CON SUBSTAGE(1) 2 minutes, room temperature
SUBSTAGE(2) 15 hours, room temperature -> 60 deg C
SUBSTAGE(3) 60 deg C -> room temperature
NTE Suzuki coupling reaction

RX(139) RCT KV 875269-87-7

STAGE(1)
RGT E 1310-73-2 NaOH, KY 7722-84-1 H2O2
SOL 7732-18-5 Water, 109-99-9 THF
CON 1 hour, room temperature

STAGE(2)
RGT CC 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON pH 7.0

PRO KX 875269-88-8

RX(140) RCT KE 513-38-2, KX 875269-88-8
RGT AH 534-17-8 Cs2CO3
PRO KZ 875269-89-9
SOL 68-12-2 DMF
CON 15 hours, 90 deg C

RX(141) RCT KZ 875269-89-9
RGT C 76-05-1 F3CCO2H
PRO CS 875269-90-2
SOL 75-09-2 CH2Cl2
CON 15 hours, room temperature

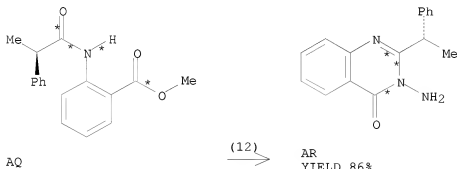
RX(33) RCT Z 75-30-9, CS 875269-90-2
RGT AH 534-17-8 Cs2CO3
PRO CT 875259-02-2
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 15 hours, room temperature -> 90 deg C
SUBSTAGE(2) 90 deg C -> room temperature

L3 ANSWER 41 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 144:166375 CASREACT
TITLE: The stereoselective synthesis of aziridine analogues
of diaminopimelic acid (DAP) and their interaction
with DAP epimerase
AUTHOR(S): Diaper, Christopher M.; Sutherland, Andrew; Pillai,
Bindu; James, Michael N. G.; Semchuk, Paul; Blanchard,

CORPORATE SOURCE: John S.; Vederas, John C.
 Department of Chemistry, University of Alberta,
 Edmonton, AB, T6G 2G2, Can.
 SOURCE: Organic & Biomolecular Chemistry (2005), 3(24),
 4402-4411
 CODEN: OBCRAK; ISSN: 1477-0520
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Aziridine analogs of diaminopimelic acid (DAP) have been prepared stereoselectively for the first time and evaluated as inhibitors of DAP epimerase. (2R,3S,3'S)-3-(3'-Aminopropane)aziridine-2,3'-dicarboxylate 4 was synthesized and shown to be a reversible inhibitor of DAP epimerase with an IC50 value of 2.88 mM. (2S,4S)- and (2S,4R)-2-(4-Amino-4-carboxybutyl)aziridine-2-carboxylic acid (LL-azi-DAP 14 and DL-azi-DAP 29) were made as pure diastereomers, and both were shown to be irreversible inhibitors of DAP epimerase. LL-Azi-DAP 14 selectively binds to Cys-73 of the enzyme active site whereas DL-azi-DAP 29 binds to Cys-217 via attack of sulfhydryl on the methylene of the inhibitor aziridine ring. These observations are consistent with the two base mechanism proposed for the epimerization of LL-DAP 1 and meso-DAP 2 by DAP epimerase.

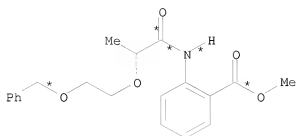
RX(12) OF 122 ...AQ ==> AR



RX(12) RCT AQ 923014-08-8
 RGT AS 7803-57-8 N2H4-H2O
 PRO AR 874534-88-0
 SOL 64-17-5 EtOH
 CON 16 hours, 140 deg C
 NTE sealed tube used

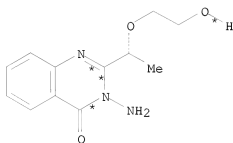
RX(13) OF 122 ...AT ==> AU...

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AT

(13)



AU

YIELD 69%

RX(13) RCT AT 445397-16-0

STAGE(1)

RGT AV 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 19 hours, room temperature

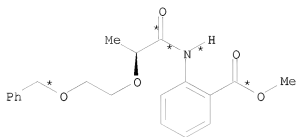
STAGE(2)

RGT AW 302-01-2 N2H4
SOL 64-17-5 EtOH
CON 2 hours, 140 deg C

PRO AU 445397-14-8

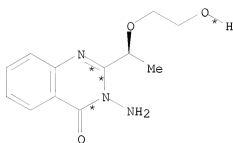
NTE sealed tube in 2nd stage

RX(14) OF 122 AY ==> AZ...



AY

(14) \longrightarrow



AZ

RX(14) RCT AY 923015-23-0

STAGE(1)

RGT AV 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 67-56-1 MeOH

CON 19 hours, room temperature

STAGE(2)

RGT AW 302-01-2 N2H4

SOL 64-17-5 EtOH

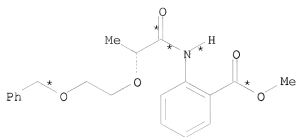
CON 2 hours, 140 deg C

PRO AZ 874534-89-1

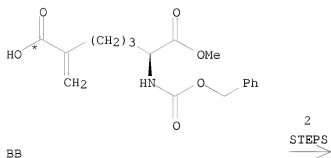
NTE sealed tube in 2nd stage

RX(44) OF 122 COMPOSED OF RX(13), RX(16)

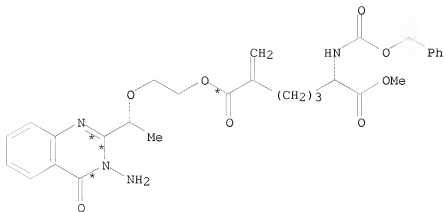
RX(44) AT + BB ==> BD



AT



BB



BD
YIELD 62%

RX(13) RCT AT 445397-16-0

STAGE(1)

RGT AV 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 19 hours, room temperature

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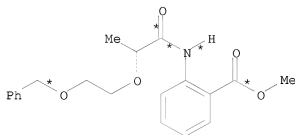
STAGE(2)

RGT AW 302-01-2 N2H4
SOL 64-17-5 EtOH
CON 2 hours, 140 deg C

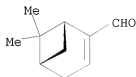
PRO AU 445397-14-8
NTE sealed tube in 2nd stage

RX(16) RCT AU 445397-14-8, BB 874534-90-4
RGT BE 538-75-0 DCC
PRO BD 874534-91-5
CAT 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
CON 1 hour, room temperature

RX(45) OF 122 COMPOSED OF RX(13), RX(32)
RX(45) AT + CG ==> CH

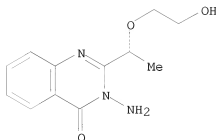


AT



CG

2
STEPS
→

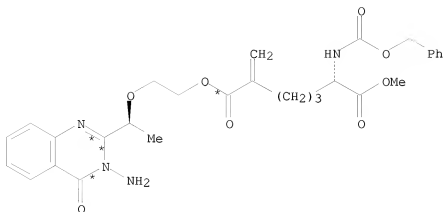


CH
YIELD 89%
(-)-Myrtenal c
onjugates

RX(13) RCT AT 445397-16-0

STAGE(1)

RGT AV 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH



BG

YIELD 51%

RX(14) RCT AY 923015-23-0

STAGE(1)

RGT AV 1333-74-0 H2

CAT 7440-05-3 Pd

SOL 67-56-1 MeOH

CON 19 hours, room temperature

STAGE(2)

RGT AW 302-01-2 N2H4

SOL 64-17-5 EtOH

CON 2 hours, 140 deg C

PRO AZ 874534-89-1

NTE sealed tube in 2nd stage

RX(18) RCT AZ 874534-89-1, BB 874534-90-4

RGT BH 64075-39-4D Benzenemethanamine, N-(cyclohexylcarbonimidoyl)-

PRO BG 874534-93-7

CAT 1122-58-3 4-DMAP

SOL 75-09-2 CH2Cl2

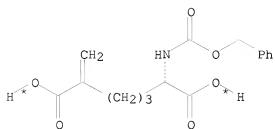
CON 48 hours, room temperature

NTE solid-supported reagent

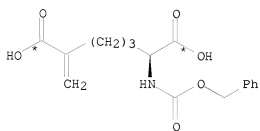
RX(73) OF 122 COMPOSED OF REACTION SEQUENCE RX(15), RX(16)
 AND REACTION SEQUENCE RX(13), RX(16)

...2 BA + 3 M ==> BB...

... AT + BB ==> BD



BA



BA

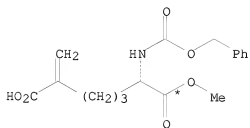


2 M



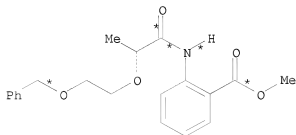
M

2
STEPS
→



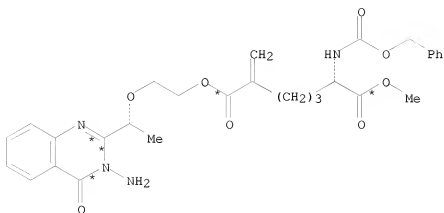
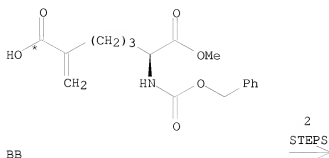
BB

START NEXT REACTION SEQUENCE



AT

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YIELD 62%

RX(15) RCT BA 874535-03-2, M 67-56-1
RGT BC 104-15-4 TsOH
PRO AF 874534-85-7, BB 874534-90-4
SOL 67-56-1 MeOH
CON 16 hours, room temperature
NTE solid-supported reagent, 100% overall yield

RX(13) RCT AT 445397-16-0

STAGE(1)
RGT AV 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 19 hours, room temperature

STAGE(2)
RGT AW 302-01-2 N2H4
SOL 64-17-5 EtOH
CON 2 hours, 140 deg C

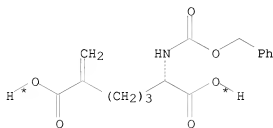
PRO AU 445397-14-8
NTE sealed tube in 2nd stage

RX(16) RCT AU 445397-14-8, BB 874534-90-4

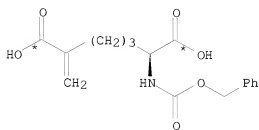
10/ 562,112

RGT BE 538-75-0 DCC
 PRO BD 874534-91-5
 CAT 1122-58-3 4-DMAP
 SOL 75-09-2 CH2C12
 CON 1 hour, room temperature

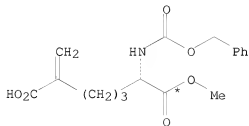
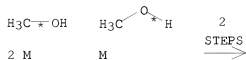
RX(77) OF 122 COMPOSED OF REACTION SEQUENCE RX(15), RX(18)
 AND REACTION SEQUENCE RX(14), RX(18)
 ...2 BA + 3 M ==> BB...
 ... AY + BB ==> BG



BA



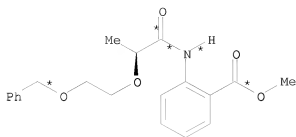
BA



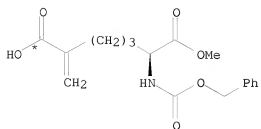
BB

START NEXT REACTION SEQUENCE

10/ 562,112

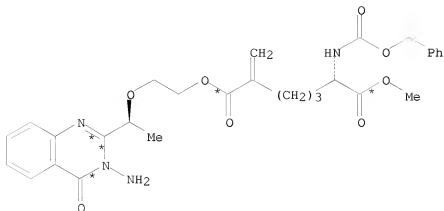


AY



BB

2
STEPS
→



BG

YIELD 51%

RX(15) RCT BA 874535-03-2, M 67-56-1
 RGT BC 104-15-4 TsOH
 PRO AF 874534-85-7, BB 874534-90-4
 SOL 67-56-1 MeOH
 CON 16 hours, room temperature
 NTE solid-supported reagent, 100% overall yield

RX(14) RCT AY 923015-23-0

STAGE(1)

RGT AV 1333-74-0 H2
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 CON 19 hours, room temperature

STAGE(2)

RGT AW 302-01-2 N2H4
 SOL 64-17-5 EtOH
 CON 2 hours, 140 deg C

PRO AZ 874534-89-1
 NTE sealed tube in 2nd stage

RX(18) RCT AZ 874534-89-1, BB 874534-90-4
 RGT BH 64075-39-4D Benzenemethanamine, N-(cyclohexylcarbonimidoyl)-
 PRO BG 874534-93-7
 CAT 1122-58-3 4-DMAP
 SOL 75-09-2 CH2Cl2
 CON 48 hours, room temperature
 NTE solid-supported reagent

REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 42 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:36301 CASREACT
 TITLE: Exploiting the Dual Reactivity of o-Isocyanobenzamide:

Three-Component Synthesis of
 4-Imino-4H-3,1-benzoxazines
 Bonne, Damien; Dekhane, Mouloud; Zhu, Jieping
 Institut de Chimie des Substances Naturelles, CNRS,
 Gif-sur-Yvette, 91198, Fr.

SOURCE: Organic Letters (2005), 7(23), 5285-5288

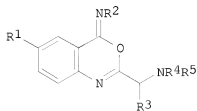
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

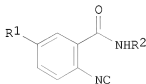
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

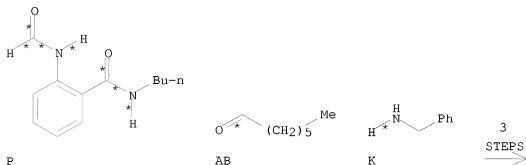


II

AB A multicomponent synthesis of 4-imino-4H-3,1-benzoxazines I [R1 = H, MeO;
 R2 = n-Bu, PhCH2, PhCH2CH2, (S)-PhCH2CH(CO2Me), etc.; R3 = H, Me2CH,
 cyclohexyl, n-hexyl; R4 = H, R5 = n-Bu, MeO2CCH2CH2, PhCH2,

9-fluorenylmethyl; R4 = R5 = Me; R4R5N = morpholino] is developed. Heating a toluene solution of an aldehyde R3CHO, an amine R4R5NH, and an isonitrile II in the presence of a stoichiometric amount of ammonium chloride at 60 °C for 12 h produces the benzoxazines I in good to excellent yields.

RX(80) OF 89 COMPOSED OF RX(8), RX(19), RX(27)
 RX(80) P + AB + K ==> BF



BF
 YIELD 65%

RX(8) RCT P 870672-07-4

STAGE(1)

RGT W 7087-68-5 EtN(Pr-i)2, X 10025-87-3 POC13
 SOL 75-09-2 CH2Cl2
 CON 2 hours, 0 deg C

STAGE(2)

RGT Y 584-08-7 K2CO3
 SOL 7732-18-5 Water

PRO V 870672-10-9

RX(19) RCT AB 111-71-7, K 100-46-9

STAGE(1)

RGT AG 12125-02-9 NH4Cl
 SOL 108-88-3 PhMe

CON 15 minutes, room temperature

STAGE(2)

RCT V 870672-10-9

CON 12 hours, 60 deg C

PRO AV 870672-20-1

RX(27) RCT AV 870672-20-1
 RGT BG 110-89-4 Piperidine
 PRO BF 870672-28-9
 SOL 141-78-6 AcOEt
 CON 4 days, 70 deg C

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 43 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 144:22759 CASREACT

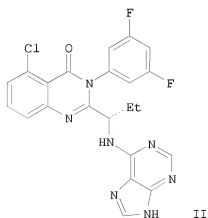
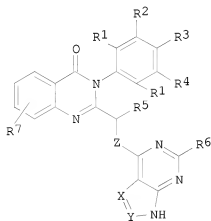
TITLE: Preparation of purine quinazolinones as inhibitors of
 human phosphatidylinositol 3-kinase delta
 INVENTOR(S): Fowler, Kerry W.; Huang, Danwen; Kesicki, Edward A.;
 Ooi, Hua Chee; Oliver, Amy R.; Ruan, Fuqiang;
 Treiberg, Jennifer

PATENT ASSIGNEE(S): Icos Corporation, USA
 SOURCE: PCT Int. Appl., 247 pp.
 CODEN: PIXXD2

DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005113556	A1	20051201	WO 2005-US16778	20050512
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005245875	A1	20051201	AU 2005-245875	20050512
CA 2566609	A1	20051201	CA 2005-2566609	20050512
WO 2005113554	A2	20051201	WO 2005-US16661	20050512
WO 2005113554	A3	20060406		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,				

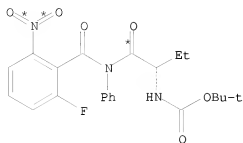
ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
 EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
 RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
 MR, NE, SN, TD, TG
 EP 1761540 A1 20070314 EP 2005-752122 20050512
 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA,
 HR, LV, MK, YU
 CN 101031569 A 20070905 CN 2005-80023449 20050512
 JP 2007537291 T 20071220 JP 2007-513402 20050512
 US 20080275067 A1 20081106 US 2007-596092 20071214
 US 2004-570784P 20040513
 PRIORITY APPLN. INFO.: WO 2005-US16778 20050512
 OTHER SOURCE(S): MARPAT 144:22759
 GI



AB Quinazolinone derivs. of formula I (X, Y = N, (substituted) CH; Z = NH, O;
 R1-R3 = H, halo, alkyl; R4 = H, halo, OH, alkoxy, CN, acyl, etc.; R5 =
 alkyl, Ph, CH2C.tplbond.CH, etc.; R6 = H, halo, (substituted) NH2; R7 =
 alkyl, halo, CF3, etc.; ZR5 = alkylene) are prepared that inhibit
 PI3Kδ activity. Methods of inhibiting phosphatidylinositol 3-kinase
 delta isoform (PI3Kδ) activity, and methods of treating diseases,
 such as disorders of immunity and inflammation in which PI3Kδ plays
 a role in leukocyte function, using the compds. also are disclosed. Thus,
 II was prepared, and had EC50 value of 1.6 nM in human B lymphocyte assay.

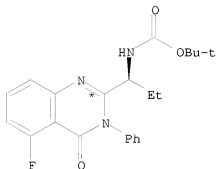
RX(110) OF 752 ...GM ==> GN...

10/ 562,112



GM

(110)
→



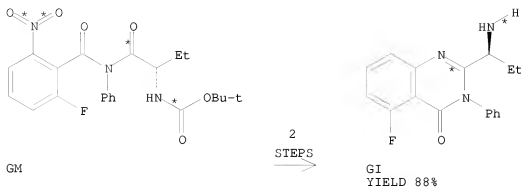
GN

YIELD 69%

RX(110) RCT GM 870281-84-8
RGT BO 7440-66-6 Zn
PRO GN 870281-85-9
SOL 64-19-7 AcOH
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) <35 deg C
SUBSTAGE(3) <35 deg C
SUBSTAGE(4) <35 deg C -> room temperature
SUBSTAGE(5) 2 hours, room temperature

RX(233) OF 752 COMPOSED OF RX(110), RX(111)

RX(233) GM ==> GI



RX(110) RCT GM 870281-84-8
 RGT BO 7440-66-6 Zn
 PRO GN 870281-85-9
 SOL 64-19-7 AcOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) <35 deg C
 SUBSTAGE(3) <35 deg C
 SUBSTAGE(4) <35 deg C -> room temperature
 SUBSTAGE(5) 2 hours, room temperature

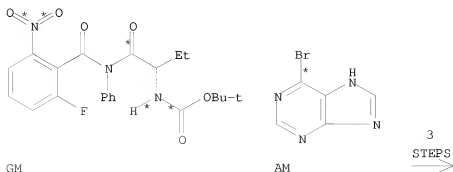
RX(111) RCT GN 870281-85-9

STAGE(1)
 RGT BJ 76-05-1 F3CCO2H
 SOL 75-09-2 CH2Cl2
 CON 1 hour, room temperature

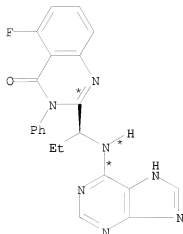
STAGE(2)
 RGT W 584-08-7 K2CO3
 SOL 7732-18-5 Water, 75-09-2 CH2Cl2
 CON room temperature, pH >10

PRO GI 870281-86-0

RX(357) OF 752 COMPOSED OF RX(110), RX(111), RX(107)
 RX(357) GM + AM ==> GJ



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GJ
YIELD 50%

RX(110) RCT GM 870281-84-8
RGT BO 7440-66-6 Zn
PRO GN 870281-85-9
SOL 64-19-7 AcOH
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) <35 deg C
SUBSTAGE(3) <35 deg C
SUBSTAGE(4) <35 deg C -> room temperature
SUBSTAGE(5) 2 hours, room temperature

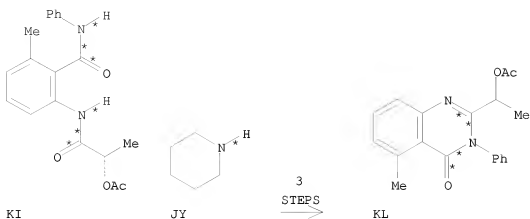
RX(111) RCT GN 870281-85-9
STAGE(1)
RGT BJ 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2
CON 1 hour, room temperature

STAGE(2)
RGT W 584-08-7 K2CO3
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON room temperature, pH >10

PRO GI 870281-86-0

RX(107) RCT GI 870281-86-0, AM 767-69-1
RGT AE 7087-68-5 EtN(Pr-i)2
PRO GJ 870281-82-6
SOL 75-65-0 t-BuOH
CON SUBSTAGE(1) room temperature -> 80 deg C
SUBSTAGE(2) 24 hours, 80 deg C

RX(448) OF 752 COMPOSED OF RX(174), RX(175), RX(176)
RX(448) KI + JY ==> KL



RX(174) RCT KI 870282-48-7

STAGE(1)

RGT AE 7087-68-5 EtN(Pr-i)2, JX 7553-56-2 I2, IO 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON 4 days, room temperature

STAGE(2)

RGT BM 144-55-8 NaHCO3

SOL 7732-18-5 Water

CON room temperature

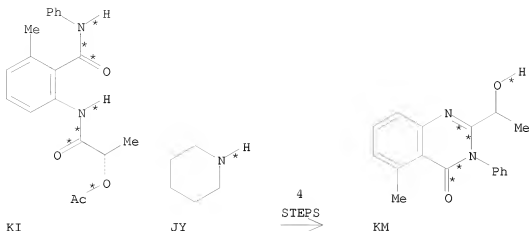
PRO KJ 870282-49-8

RX(175) RCT KJ 870282-49-8, JY 110-89-4
 PRO KK 870282-50-1
 CON 19.5 hours, room temperature
 NTE other product also detected

RX(176) RCT KK 870282-50-1
 PRO KL 870282-51-2
 SOL 75-05-8 MeCN
 CON SUBSTAGE(1) room temperature -> reflux
 SUBSTAGE(2) 3 hours, reflux

RX(451) OF 752 COMPOSED OF RX(174), RX(175), RX(176), RX(177)

RX(451) KI + JY ==> KM



RX(174) RCT KI 870282-48-7

STAGE(1)

RGT AE 7087-68-5 EtN(Pr-i)2, JX 7553-56-2 I2, IO 603-35-0 PPh3
 SOL 75-09-2 CH2Cl2
 CON 4 days, room temperature

STAGE(2)

RGT BM 144-55-8 NaHCO3
 SOL 7732-18-5 Water
 CON room temperature

PRO KJ 870282-49-8

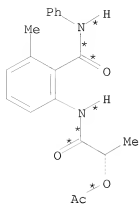
RX(175) RCT KJ 870282-49-8, JY 110-89-4
 PRO KK 870282-50-1
 CON 19.5 hours, room temperature
 NTE other product also detected

RX(176) RCT KK 870282-50-1
 PRO KL 870282-51-2
 SOL 75-05-8 MeCN
 CON SUBSTAGE(1) room temperature -> reflux
 SUBSTAGE(2) 3 hours, reflux

RX(177) RCT KL 870282-51-2
 RGT W 584-08-7 K2CO3
 PRO KM 870282-52-3
 SOL 67-56-1 MeOH
 CON 20 minutes, room temperature

RX(723) OF 752 COMPOSED OF RX(174), RX(175), RX(176), RX(177), RX(178)

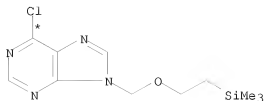
RX(723) KI + JY + AV ==> KF



KI

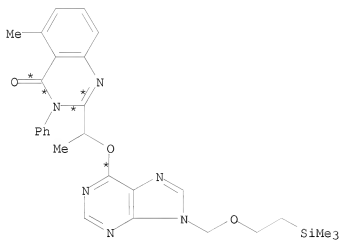


JY



AV

5
STEPS
→



KF

RX(174) RCT KI 870282-48-7

STAGE(1)

RGT AE 7087-68-5 EtN(Pr-i)₂, JX 7553-56-2 I₂, IO 603-35-0 PPh₃
 SOL 75-09-2 CH₂Cl₂
 CON 4 days, room temperature

STAGE(2)

RGT BM 144-55-8 NaHCO₃
 SOL 7732-18-5 Water
 CON room temperature

PRO KJ 870282-49-8

RX(175) RCT KJ 870282-49-8, JY 110-89-4
 PRO KK 870282-50-1
 CON 19.5 hours, room temperature
 NTE other product also detected

RX(176) RCT KK 870282-50-1
 PRO KL 870282-51-2
 SOL 75-05-8 MeCN
 CON SUBSTAGE(1) room temperature -> reflux
 SUBSTAGE(2) 3 hours, reflux

RX(177) RCT KL 870282-51-2
 RGT W 584-08-7 K₂CO₃
 PRO KM 870282-52-3
 SOL 67-56-1 MeOH
 CON 20 minutes, room temperature

RX(178) RCT KM 870282-52-3

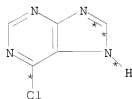
STAGE(1)
 RGT KN 7646-69-7 NaH
 SOL 109-99-9 THF
 CON 10 minutes, room temperature

STAGE(2)
 RCT AV 222296-31-3
 SOL 109-99-9 THF
 CON SUBSTAGE(1) 21.5 hours, room temperature
 SUBSTAGE(2) 1.5 hours, room temperature
 SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
 RGT KO 12125-02-9 NH₄Cl
 SOL 7732-18-5 Water
 CON room temperature

PRO KF 870282-53-4

RX(727) OF 752 COMPOSED OF REACTION SEQUENCE RX(13), RX(178)
 AND REACTION SEQUENCE RX(174), RX(175), RX(176), RX(177),
 RX(178)
 ...AU + AN ==> AV...
 ... KI + JY + AV ==> KF



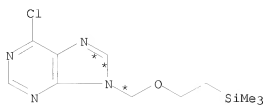
AU



AN

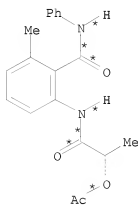
5
 STEPS
 →

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AV

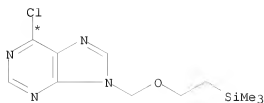
START NEXT REACTION SEQUENCE



KI

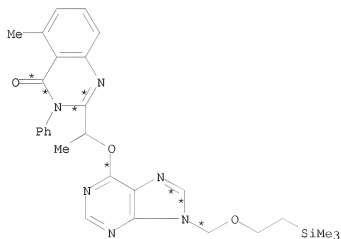


JY



AV

5
STEPS
→



KF

RX(13)	RCT	AU 87-42-3, AN 76513-69-4
	RGT	W 584-08-7 K2CO3
	PRO	AV 222296-31-3
	SOL	68-12-2 DMF
	CON	18 hours, room temperature

NTE mol. sieves used

RX(174) RCT KI 870282-48-7

STAGE(1)

RGT AE 7087-68-5 EtN(Pr-i)2, JX 7553-56-2 I2, IO 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON 4 days, room temperature

STAGE(2)

RGT BM 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON room temperature

PRO KJ 870282-49-8

RX(175) RCT KJ 870282-49-8, JY 110-89-4

PRO KK 870282-50-1
CON 19.5 hours, room temperature
NTE other product also detected

RX(176) RCT KK 870282-50-1

PRO KL 870282-51-2
SOL 75-05-8 MeCN
CON SUBSTAGE(1) room temperature -> reflux
SUBSTAGE(2) 3 hours, reflux

RX(177) RCT KL 870282-51-2

RGT W 584-08-7 K2CO3
PRO KM 870282-52-3
SOL 67-56-1 MeOH
CON 20 minutes, room temperature

RX(178) RCT KM 870282-52-3

STAGE(1)

RGT KN 7646-69-7 NaH
SOL 109-99-9 THF
CON 10 minutes, room temperature

STAGE(2)

RCT AV 222296-31-3
SOL 109-99-9 THF
CON SUBSTAGE(1) 21.5 hours, room temperature
SUBSTAGE(2) 1.5 hours, room temperature
SUBSTAGE(3) 1 hour, room temperature

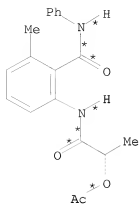
STAGE(3)

RGT KO 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON room temperature

PRO KF 870282-53-4

RX(728) OF 752 COMPOSED OF RX(174), RX(175), RX(176), RX(177), RX(178), RX(172)

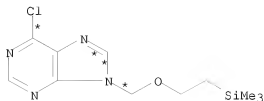
RX(728) KI + JY + AV ==> KG



KI

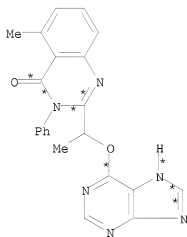


JY



AV

6
STEPS
→



KG

RX(174) RCT KI 870282-48-7

STAGE(1)

RGT AE 7087-68-5 EtN(Pr-i)2, JX 7553-56-2 I2, IO 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON 4 days, room temperature

STAGE(2)

RGT BM 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON room temperature

PRO KJ 870282-49-8

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RX(175)  RCT  KJ 870282-49-8, JY 110-89-4
          PRO  KK 870282-50-1
          CON  19.5 hours, room temperature
          NTE  other product also detected

RX(176)  RCT  KK 870282-50-1
          PRO  KL 870282-51-2
          SOL  75-05-8 MeCN
          CON  SUBSTAGE(1) room temperature -> reflux
          SUBSTAGE(2) 3 hours, reflux

RX(177)  RCT  KL 870282-51-2
          RGT  W 584-08-7 K2CO3
          PRO  KM 870282-52-3
          SOL  67-56-1 MeOH
          CON  20 minutes, room temperature

RX(178)  RCT  KM 870282-52-3

          STAGE(1)
          RGT  KN 7646-69-7 NaH
          SOL  109-99-9 THF
          CON  10 minutes, room temperature

          STAGE(2)
          RCT  AV 222296-31-3
          SOL  109-99-9 THF
          CON  SUBSTAGE(1) 21.5 hours, room temperature
          SUBSTAGE(2) 1.5 hours, room temperature
          SUBSTAGE(3) 1 hour, room temperature

          STAGE(3)
          RGT  KO 12125-02-9 NH4Cl
          SOL  7732-18-5 Water
          CON  room temperature

          PRO  KF 870282-53-4

RX(172)  RCT  KF 870282-53-4

          STAGE(1)
          RGT  AH 7647-01-0 HCl
          SOL  7732-18-5 Water, 67-56-1 MeOH
          CON  SUBSTAGE(1) room temperature -> 40 deg C
          SUBSTAGE(2) 3 hours, 40 deg C
          SUBSTAGE(3) cooled

          STAGE(2)
          RGT  W 584-08-7 K2CO3
          SOL  7732-18-5 Water
          CON  room temperature, pH 10

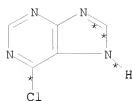
          PRO  KG 870282-47-6

RX(734)  OF  752 COMPOSED OF REACTION SEQUENCE RX(13), RX(178), RX(172)
          AND REACTION SEQUENCE RX(174), RX(175), RX(176), RX(177),
          RX(178), RX(172)
...AU + AN ==> AV...

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... KI + JY + AV ==> KG

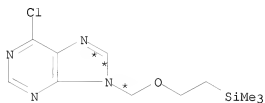


AU



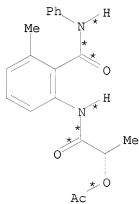
AN

6
STEPS
→



AV

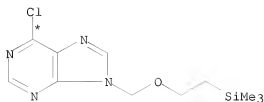
START NEXT REACTION SEQUENCE



KI

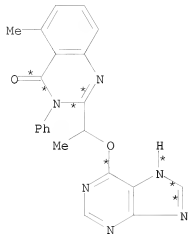


JY



AV

6
STEPS
→



KG

RX(13) RCT AU 87-42-3, AN 76513-69-4
 RGT W 584-08-7 K2CO3
 PRO AV 222296-31-3
 SOL 68-12-2 DMF
 CON 18 hours, room temperature
 NTE mol. sieves used

RX(174) RCT KI 870282-48-7

STAGE(1)

RGT AE 7087-68-5 EtN(Pr-i)2, JX 7553-56-2 I2, IO 603-35-0 PPh3
 SOL 75-09-2 CH2Cl2
 CON 4 days, room temperature

STAGE(2)

RGT BM 144-55-8 NaHCO3
 SOL 7732-18-5 Water
 CON room temperature

PRO KJ 870282-49-8

RX(175) RCT KJ 870282-49-8, JY 110-89-4
 PRO KK 870282-50-1
 CON 19.5 hours, room temperature
 NTE other product also detected

RX(176) RCT KK 870282-50-1
 PRO KL 870282-51-2
 SOL 75-05-8 MeCN
 CON SUBSTAGE(1) room temperature -> reflux
 SUBSTAGE(2) 3 hours, reflux

RX(177) RCT KL 870282-51-2
 RGT W 584-08-7 K2CO3
 PRO KM 870282-52-3
 SOL 67-56-1 MeOH
 CON 20 minutes, room temperature

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RX(178) RCT KM 870282-52-3

STAGE(1)

RGT KN 7646-69-7 NaH
SOL 109-99-9 THF
CON 10 minutes, room temperature

STAGE(2)

RCT AV 222296-31-3
SOL 109-99-9 THF
CON SUBSTAGE(1) 21.5 hours, room temperature
SUBSTAGE(2) 1.5 hours, room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

RGT KO 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON room temperature

PRO KF 870282-53-4

RX(172) RCT KF 870282-53-4

STAGE(1)

RGT AH 7647-01-0 HCl
SOL 7732-18-5 Water, 67-56-1 MeOH
CON SUBSTAGE(1) room temperature -> 40 deg C
SUBSTAGE(2) 3 hours, 40 deg C
SUBSTAGE(3) cooled

STAGE(2)

RGT W 584-08-7 K2CO3
SOL 7732-18-5 Water
CON room temperature, pH 10

PRO KG 870282-47-6

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 44 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 143:460174 CASREACT

TITLE: Preparation of heterocyclic amides as MMP-13
inhibitors for treating osteoarthritis and rheumatoid
arthritis

INVENTOR(S): Terauchi, Jun; Kuno, Haruhiko; Nara, Hiroshi; Oki,
Hideyuki; Sato, Kenjiro

PATENT ASSIGNEE(S): Takeda Pharmaceutical Company Limited, Japan

SOURCE: PCT Int. Appl., 455 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

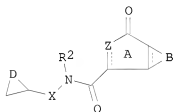
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2005238386	A1	20051110	AU 2005-238386	20050428
CA 2564085	A1	20051110	CA 2005-2564085	20050428
EP 1740551	A1	20070110	EP 2005-739012	20050428
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU			
CN 1976907	A	20070606	CN 2005-80021727	20050428
BR 2005010305	A	20071002	BR 2005-10305	20050428
JP 2007535488	T	20071206	JP 2006-540833	20050428
MX 2006012333	A	20070117	MX 2006-12333	20061025
US 20080027050	A1	20080131	US 2006-579298	20061030
IN 2006KN03427	A	20070615	IN 2006-KN3427	20061120
KR 2007008709	A	20070117	KR 2006-724701	20061124
NO 2006005537	A	20070129	NO 2006-5537	20061130
PRIORITY APPLN. INFO.:			JP 2004-135596	20040430
			WO 2005-JP8549	20050428

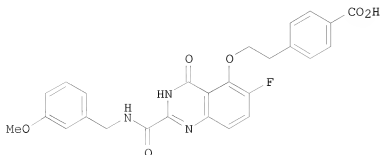
OTHER SOURCE(S): MARPAT 143:460174
GI



I



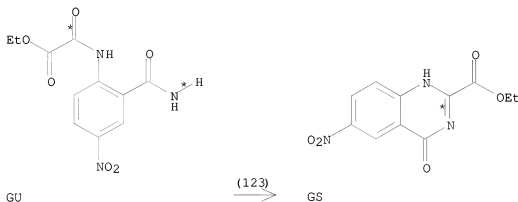
II



III

AB The invention is related to the preparation of heterocyclic amides of formula I [A = (un)substituted N-containing heterocycle; B = (un)substituted monocyclic homocycle or heterocycle; Z = N, NH and derivs.; R2 = H, (un)substituted hydrocarbyl; X = (un)substituted spacer; D = (un)substituted heterocycle other than II; X' = S, O, SO, CH2; and at least one of B and C has substituent(s); with the exception of 2 compds.; their salts, and their prodrugs] having a matrix metalloproteinase, particularly MMP-13, inhibitory activity. Thus, reacting 5,6-difluoro-N-[[3-(methyloxy)phenyl]methyl]-4-oxo-3,4-dihydroquinazoline-2-carboxamide (preparation given) with 4-(2-hydroxyethyl)benzoic acid gave amide III in 70% yield. III displayed an inhibitory rate of 99% towards MMP-13 activity. I are useful for treating osteoarthritis and rheumatoid arthritis.

RX(123) OF 1000 GU ==> GS...



RX(123) RCT GU 54166-78-8

STAGE(1)

RGT FB 141-52-6 NaOEt
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> room temperature
 SUBSTAGE(3) 12 hours, room temperature

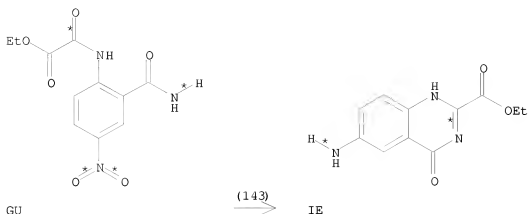
STAGE(2)

RGT GV 77-92-9 Citric acid
 SOL 7732-18-5 Water
 CON room temperature

PRO GS 34632-65-0

RX(143) OF 1000 GU ==> IE...

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RX(143) RCT GU 54166-78-8

STAGE(1)

RGT CI 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH, 109-99-9 THF
CON 8 hours, room temperature

STAGE(2)

RGT FB 141-52-6 NaOEt
SOL 64-17-5 EtOH, 109-99-9 THF
CON 12 hours, room temperature

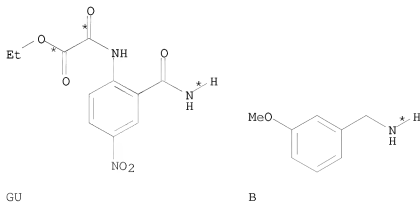
STAGE(3)

RGT GV 77-92-9 Citric acid
SOL 7732-18-5 Water
CON room temperature

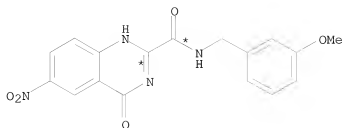
PRO IE 34632-66-1

RX(725) OF 1000 COMPOSED OF RX(123), RX(122)

RX(725) GU + B \implies GT



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GT

RX(123) RCT GU 54166-78-8

STAGE(1)

RGT FB 141-52-6 NaOEt

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 0 deg C -> room temperature

SUBSTAGE(3) 12 hours, room temperature

STAGE(2)

RGT GV 77-92-9 Citric acid

SOL 7732-18-5 Water

CON room temperature

PRO GS 34632-65-0

RX(122) RCT B 5071-96-5, GS 34632-65-0

RGT D 121-44-8 Et3N

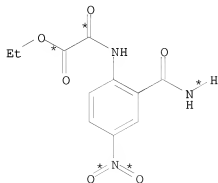
PRO GT 869294-63-3

SOL 109-99-9 THF

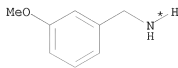
CON overnight, room temperature

RX(740) OF 1000 COMPOSED OF RX(143), RX(144)

RX(740) GU + B ==> IF

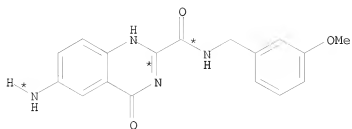


GU



B

2
STEPS
→



IF

RX(143) RCT GU 54166-78-8

STAGE(1)

RGT CI 1333-74-0 H2
 CAT 7440-05-3 Pd
 SOL 64-17-5 EtOH, 109-99-9 THF
 CON 8 hours, room temperature

STAGE(2)

RGT FB 141-52-6 NaOEt
 SOL 64-17-5 EtOH, 109-99-9 THF
 CON 12 hours, room temperature

STAGE(3)

RGT GV 77-92-9 Citric acid
 SOL 7732-18-5 Water
 CON room temperature

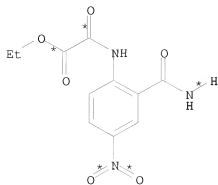
PRO IE 34632-66-1

RX(144) RCT B 5071-96-5, IE 34632-66-1
 RGT D 121-44-8 Et3N
 PRO IF 869294-81-5
 SOL 109-99-9 THF
 CON overnight, room temperature

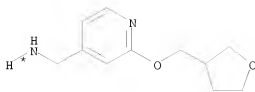
RX(741) OF 1000 COMPOSED OF RX(143), RX(145)

RX(741) GU + AD ==> IG

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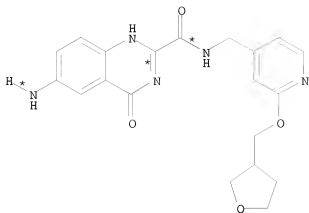


GU



AD

2
STEPS
→



IG

RX (143) RCT GU 54166-78-8

STAGE(1)

RGT CI 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH, 109-99-9 THF
CON 8 hours, room temperature

STAGE(2)

RGT FB 141-52-6 NaOEt
SOL 64-17-5 EtOH, 109-99-9 THF
CON 12 hours, room temperature

STAGE(3)

RGT GV 77-92-9 Citric acid
SOL 7732-18-5 Water
CON room temperature

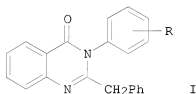
PRO IE 34632-66-1

RX(145) RCT AD 869293-60-7, IE 34632-66-1
 RGT D 121-44-8 Et3N
 PRO IG 869294-82-6
 SOL 109-99-9 THF
 CON overnight, room temperature

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

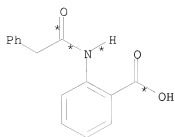
L3 ANSWER 45 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 143:367264 CASREACT
 TITLE: Green chemical multicomponent one-pot synthesis of fluorinated 2,3-disubstituted quinazolin-4(3H)-ones under solvent-free conditions and their antifungal activity
 AUTHOR(S): Dandia, Anshu; Singh, Ruby; Sarawgi, Pritima
 CORPORATE SOURCE: Department of Chemistry, University of Rajasthan, Jaipur, 302004, India
 SOURCE: Journal of Fluorine Chemistry (2005), 126(3), 307-312
 CODEN: JFLCAR; ISSN: 0022-1139
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

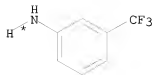


AB A rapid one-pot solvent-free procedure has been developed for the synthesis of fluorinated 2,3-disubstituted quinazolin-4(3H)-ones, e.g., I (R = 2-F, 3-F, 4-F, 2-CF₃, 3-CF₃), by neat three-component cyclocondensation of anthranilic acid, phenylacetyl chloride and substituted anilines under microwave irradiation. The exptl. methodol. and microwave conditions described here are well established, allowing significant rate enhancement and good yields compared to conventional reaction conditions. The reaction is generalized for o-, m- and p-substituted anilines with electron-donating and -withdrawing groups to give quinazolin-4(3H)-ones. The synthesized compds. have been screened for their antifungal activity.

RX(1) OF 11 A + B ==> C

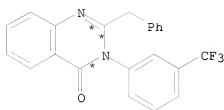


A



B

(1) →



C

YIELD 88%

RX(1) RCT A 28565-98-2

STAGE(1)

RGT D 1318-93-0 Montmorillonite, E 108-24-7 Ac2O

CON 3 minutes, 141 deg C

STAGE(2)

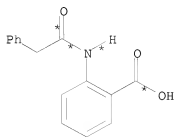
RCT B 98-16-8

CON 7 minutes, 141 deg C

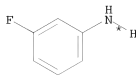
PRO C 848085-19-8

NTE green chemistry, green chemistry-process simplification,
microwave irradiation, no solvent, solid-supported reagent

RX(2) OF 11 A + F ==> G

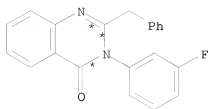


A



F

(2) →



G
YIELD 82%

RX(2) RCT A 28565-98-2

STAGE(1)

RGT D 1318-93-0 Montmorillonite, E 108-24-7 Ac2O
CON 3 minutes, 142 deg C

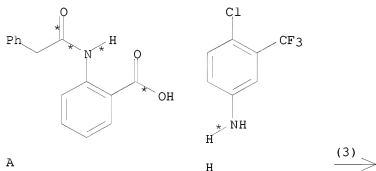
STAGE(2)

RCT F 372-19-0
CON 6 minutes, 142 deg C

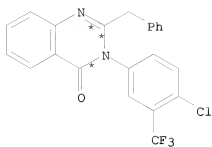
PRO G 848085-20-1

NTE green chemistry, green chemistry-process simplification,
microwave irradiation, no solvent, solid-supported reagent

RX(3) OF 11 A + H ==> I



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I
YIELD 81%

RX(3) RCT A 28565-98-2

STAGE(1)

RGT D 1318-93-0 Montmorillonite, E 108-24-7 Ac2O
CON 3 minutes, 137 deg C

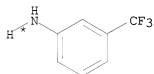
STAGE(2)

RCT H 320-51-4
CON 7 minutes, 137 deg C

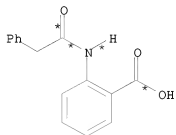
PRO I 848085-21-2

NTE green chemistry, green chemistry-process simplification,
microwave irradiation, no solvent, solid-supported reagent

RX(10) OF 11 B + A ==> C



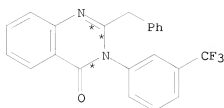
B



A

(10)
→

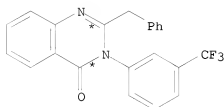
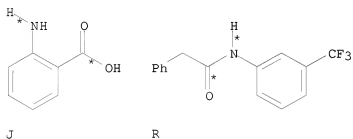
10/ 562,112



C
YIELD 91%

RX(10) RCT B 98-16-8, A 28565-98-2
PRO C 848085-19-8
CON 4 minutes, 162 deg C
NTE green chemistry, green chemistry-process simplification,
microwave irradiation, no solvent

RX(11) OF 11 J + R ==> C

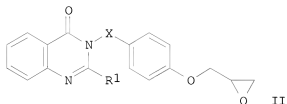
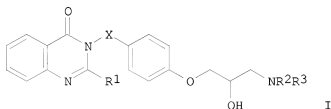


C
YIELD 90%

RX(11) RCT J 118-92-3, R 1939-21-5
PRO C 848085-19-8
CON 5 minutes, 164 deg C
NTE green chemistry, green chemistry-process simplification,
microwave irradiation, no solvent

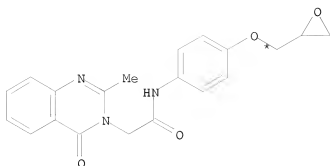
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 46 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 143:286363 CASREACT
 TITLE: Synthesis of certain (heterocyclic substituted aryloxy) propanolamines as potential adrenoceptor antagonists
 AUTHOR(S): Khalil, N. A.; Botros, S.; Soliman, L. N.; Amin, F. M.; El-Zanfaly, S.
 CORPORATE SOURCE: Organic Chemistry Department, Faculty of Pharmacy, Cairo University, Cairo, Egypt
 SOURCE: Bulletin of the Faculty of Pharmacy (Cairo University) (2002), 40(1), 23-29
 CODEN: BFPHA8; ISSN: 1110-0931
 PUBLISHER: Cairo University, Faculty of Pharmacy
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Amino(hydroxy)-functionalized quinazolinones I [X = nothing, CH₂CONH; R₁ = H, Me; R₂ = H, R₃ = n-Pr, Me₂CH, Me₃C, cyclohexyl, PhCH₂, PhCH₂CH₂; R₂ = R₃ = Et, PhCH₂; R₂R₃N = 1-pyrrolidinyl, 4-morpholinyl, 1-piperidinyl, 4-(4-methoxyphenyl)-1-piperazinyl, etc.] were prepared by ring opening of epoxides II with the corresponding primary and secondary amines. Pharmacol. screening showed that I (X = nothing; R₁ = Me; R₂ = H; R₃ = n-Bu, PhCH₂CH₂), I (X = CH₂CONH; R₁ = H; R₂ = R₃ = Et; R₂ = H, R₃ = PhCH₂) and I (X = CH₂CONH; R₁ = Me; R₂ = H; R₃ = Me₂CH) exhibited β -adrenergic blocking activity and antagonized the stimulant effect of isoprenaline on isolated frog heart.

RX(12) OF 57 ...Z + AD ==> AE...

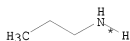


AH

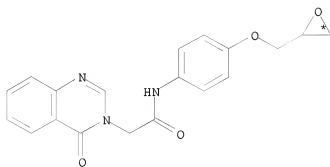
YIELD 78%

RX(13) RCT AC 864234-48-0, AD 106-89-8
 RGT AF 1310-58-3 KOH
 PRO AH 864234-50-4
 SOL 7732-18-5 Water
 CON overnight, room temperature

RX(14) OF 57 ...M + AE ==> AI

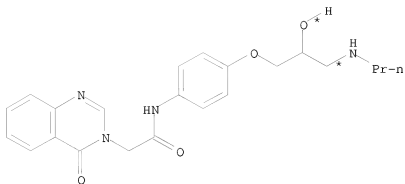


M



AE

(14) →

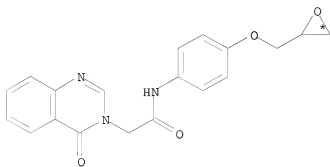


AI

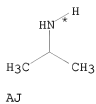
YIELD 36%

RX(14) RCT M 107-10-8, AE 864234-49-1
 PRO AI 864234-51-5
 CON 6 hours, reflux
 NTE no solvent

RX(15) OF 57 ...AE + AJ ==> AK

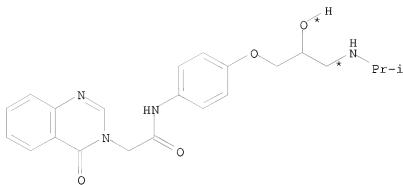


AE



AJ

(15)

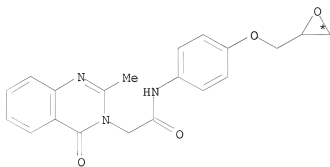


AK

YIELD 30%

RX(15) RCT AE 864234-49-1, AJ 75-31-0
 PRO AK 864234-52-6
 SOL 68-12-2 DMF
 CON 6 hours, reflux

RX(16) OF 57 ...AH + AJ ==> AM

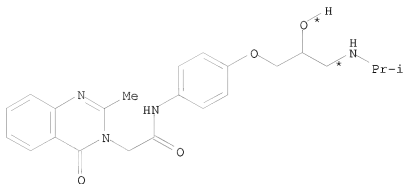


AH



AJ

(16)

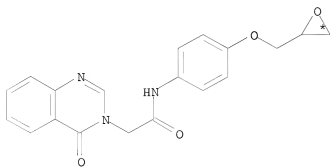


AM

YIELD 32%

RX(16) RCT AH 864234-50-4, AJ 75-31-0
 PRO AM 864234-53-7
 SOL 68-12-2 DMF
 CON 6 hours, reflux

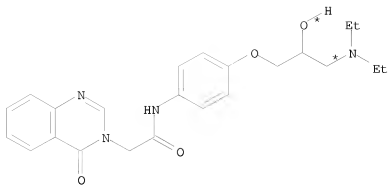
RX(17) OF 57 ...AE + F ==> AN



AE



(17) \longrightarrow

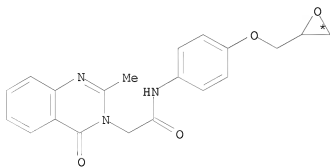


AN

YIELD 28%

RX(17) RCT AE 864234-49-1, F 109-89-7
 PRO AN 864234-54-8
 SOL 68-12-2 DMF
 CON 6 hours, reflux

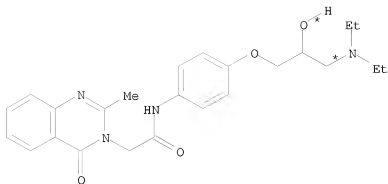
RX(18) OF 57 ...AH + F ==> AO



AH



(18) \longrightarrow

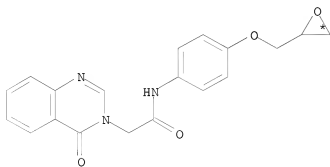


AO

YIELD 35%

RX(18) RCT AH 864234-50-4, F 109-89-7
 PRO AO 864234-55-9
 SOL 68-12-2 DMF
 CON 6 hours, reflux

RX(19) OF 57 ...AE + AP ==> AQ

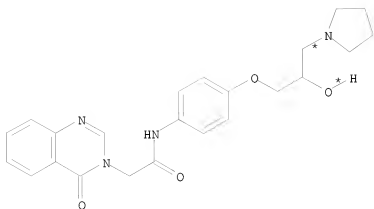


AE



AP

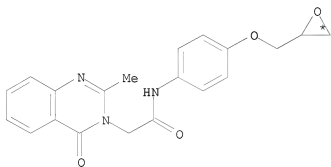
(19) →



AQ
YIELD 36%

RX(19) RCT AE 864234-49-1, AP 123-75-1
 PRO AQ 864234-56-0
 CON 6 hours, reflux
 NIE no solvent

RX(20) OF 57 ...AH + AP ==> AR

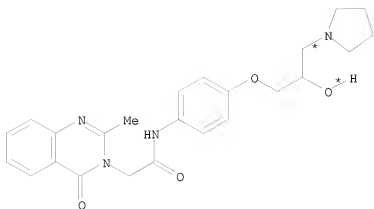


AH



AP

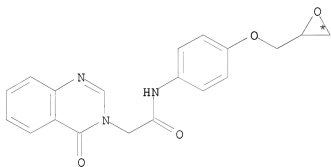
(20)
→



AR
YIELD 42%

RX(20) RCT AH 864234-50-4, AP 123-75-1
 PRO AR 864234-57-1
 CON 6 hours, reflux
 NTE no solvent

RX(21) OF 57 ...AE + AS ==> AT



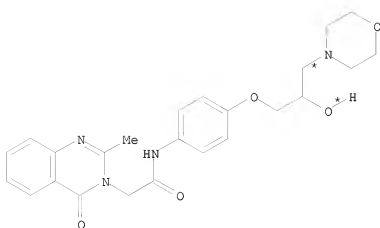
AE



AS

(21)
→

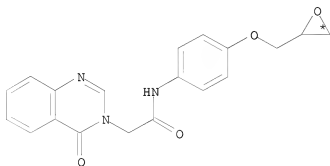
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AU
YIELD 20%

RX(22) RCT AH 864234-50-4, AS 110-91-8
 PRO AU 864234-59-3
 CON 6 hours, reflux
 NTE no solvent

RX(23) OF 57 ...AE + AV ==> AW

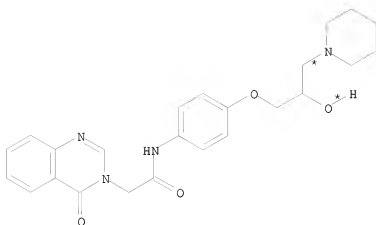


AE



AV

(23)
→

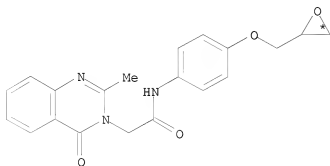


AW

YIELD 45%

RX(23) RCT AE 864234-49-1, AV 110-89-4
 PRO AW 864234-60-6
 CON 6 hours, reflux
 NTE no solvent

RX(24) OF 57 ...AH + AV ==> AX

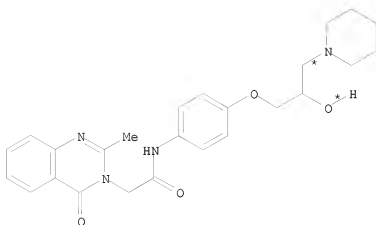


AH



AV

(24) \longrightarrow

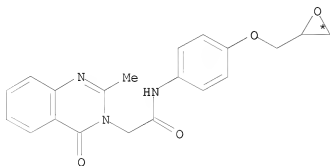


AX

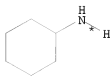
YIELD 35%

RX(24) RCT AH 864234-50-4, AV 110-89-4
 PRO AX 864234-61-7
 CON 6 hours, reflux
 NTE no solvent

RX(25) OF 57 ...AH + AY ==> AZ

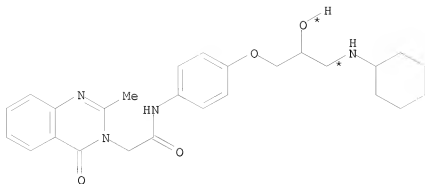


AH



AY

(25) \longrightarrow



AZ

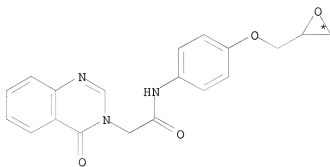
YIELD 32%

RX(25) RCT AH 864234-50-4, AY 108-91-8
 PRO AZ 864234-62-8
 CON 6 hours, reflux
 NTE no solvent

RX(26) OF 57 ...B + AE ==> BA

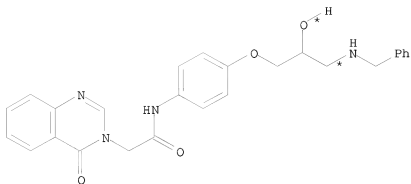


B



AE

(26) →



BA

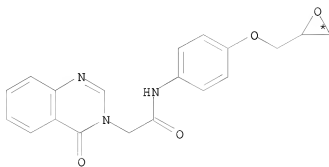
YIELD 40%

RX(26) RCT B 100-46-9, AE 864234-49-1
 PRO BA 864234-63-9
 CON 6 hours, reflux
 NTE no solvent

RX(27) OF 57 ...K + AE ==> BB

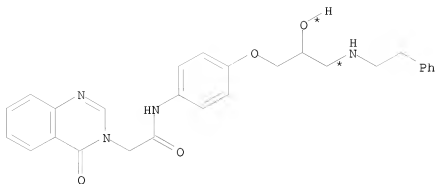


K



AE

(27)

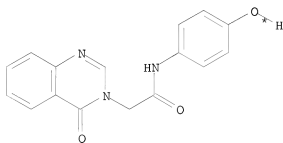


BB

YIELD 25%

RX(27) RCT K 64-04-0, AE 864234-49-1
 PRO BB 864234-64-0
 CON 6 hours, reflux
 NTE no solvent

RX(30) OF 57 COMPOSED OF RX(12), RX(14)
 RX(30) Z + AD + M ==> AI



Z

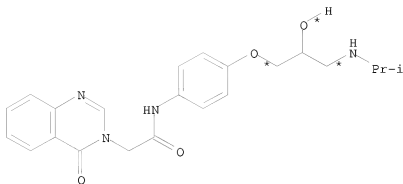


AD



M

2
 STEPS
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AK

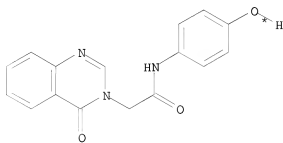
YIELD 30%

RX(12) RCT Z 591213-29-5, AD 106-89-8
 RGT AF 1310-58-3 KOH
 PRO AE 864234-49-1
 SOL 7732-18-5 Water
 CON overnight, room temperature

RX(15) RCT AE 864234-49-1, AJ 75-31-0
 PRO AK 864234-52-6
 SOL 68-12-2 DMF
 CON 6 hours, reflux

RX(32) OF 57 COMPOSED OF RX(12), RX(17)

RX(32) Z + AD + F ==> AN



Z

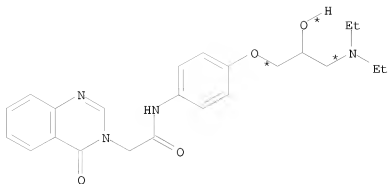


AD



F

2
 STEPS
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AN

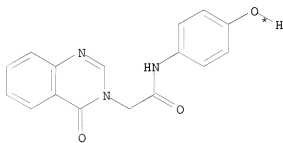
YIELD 28%

RX(12) RCT Z 591213-29-5, AD 106-89-8
RGT AF 1310-58-3 KOH
PRO AE 864234-49-1
SOL 7732-18-5 Water
CON overnight, room temperature

RX(17) RCT AE 864234-49-1, F 109-89-7
PRO AN 864234-54-8
SOL 68-12-2 DMF
CON 6 hours, reflux

RX(33) OF 57 COMPOSED OF RX(12), RX(19)

RX(33) Z + AD + AP ==> AQ



Z



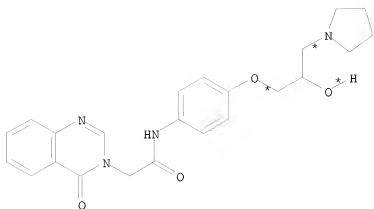
AD



AP

2
STEPS
→

10/ 562,112

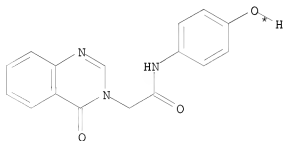


AQ
YIELD 36%

RX(12) RCT Z 591213-29-5, AD 106-89-8
 RGT AF 1310-58-3 KOH
 PRO AE 864234-49-1
 SOL 7732-18-5 Water
 CON overnight, room temperature

RX(19) RCT AE 864234-49-1, AP 123-75-1
 PRO AQ 864234-56-0
 CON 6 hours, reflux
 NTE no solvent

RX(34) OF 57 COMPOSED OF RX(12), RX(21)
RX(34) Z + AD + AS ==> AT



Z

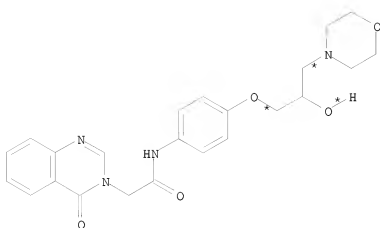


AD



AS

2
STEPS
→

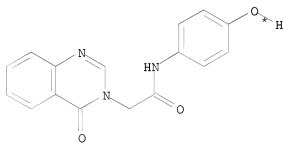


AT
YIELD 30%

RX(12) RCT Z 591213-29-5, AD 106-89-8
RGT AF 1310-58-3 KOH
PRO AE 864234-49-1
SOL 7732-18-5 Water
CON overnight, room temperature

RX(21) RCT AE 864234-49-1, AS 110-91-8
PRO AT 864234-58-2
CON 6 hours, reflux
NTE no solvent

RX(35) OF 57 COMPOSED OF RX(12), RX(23)
RX(35) Z + AD + AV ==> AW



Z

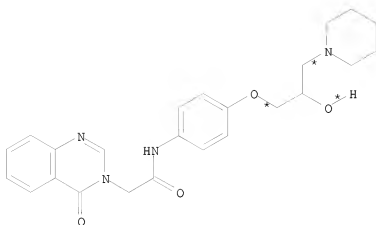


AD



AV

2
STEPS
→

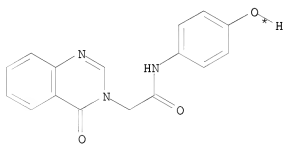


AW
YIELD 45%

RX(12) RCT Z 591213-29-5, AD 106-89-8
RGT AF 1310-58-3 KOH
PRO AE 864234-49-1
SOL 7732-18-5 Water
CON overnight, room temperature

RX(23) RCT AE 864234-49-1, AV 110-89-4
PRO AW 864234-60-6
CON 6 hours, reflux
NTE no solvent

RX(36) OF 57 COMPOSED OF RX(12), RX(26)
RX(36) Z + AD + B ==> BA



Z

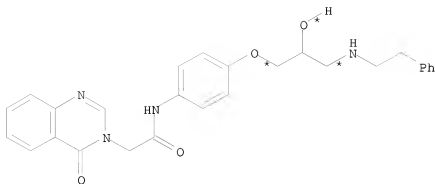


AD



B

2
STEPS
→



BB

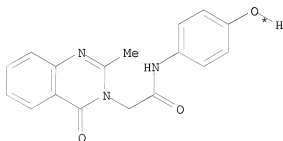
YIELD 25%

RX(12) RCT Z 591213-29-5, AD 106-89-8
 RGT AF 1310-58-3 KOH
 PRO AE 864234-49-1
 SOL 7732-18-5 Water
 CON overnight, room temperature

RX(27) RCT K 64-04-0, AE 864234-49-1
 PRO BB 864234-64-0
 CON 6 hours, reflux
 NTE no solvent

RX(38) OF 57 COMPOSED OF RX(13), RX(16)

RX(38) AC + AD + AJ ==> AM



AC

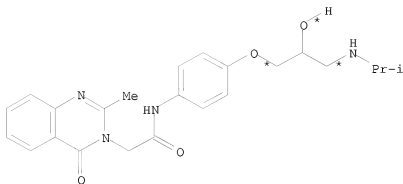


AD



AJ

2
 STEPS
 →



AM

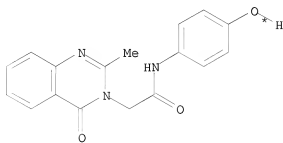
YIELD 32%

RX(13) RCT AC 864234-48-0, AD 106-89-8
 RGT AF 1310-58-3 KOH
 PRO AH 864234-50-4
 SOL 7732-18-5 Water
 CON overnight, room temperature

RX(16) RCT AH 864234-50-4, AJ 75-31-0
 PRO AM 864234-53-7
 SOL 68-12-2 DMF
 CON 6 hours, reflux

RX(39) OF 57 COMPOSED OF RX(13), RX(18)

RX(39) AC + AD + F ==> AO



AC

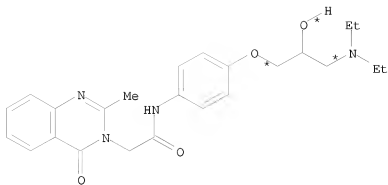


AD



F

2
 STEPS
 →



AO

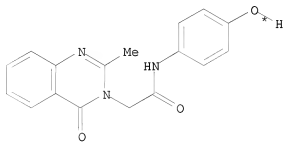
YIELD 35%

RX(13) RCT AC 864234-48-0, AD 106-89-8
RGT AF 1310-58-3 KOH
PRO AH 864234-50-4
SOL 7732-18-5 Water
CON overnight, room temperature

RX(18) RCT AH 864234-50-4, F 109-89-7
PRO AO 864234-55-9
SOL 68-12-2 DMF
CON 6 hours, reflux

RX(40) OF 57 COMPOSED OF RX(13), RX(20)

RX(40) AC + AD + AP ==> AR



AC



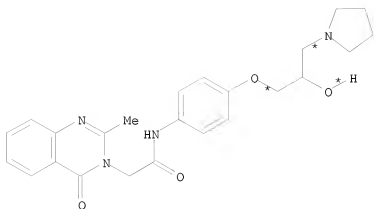
AD



AP

2
STEPS
→

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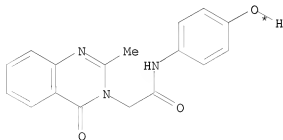


AR
YIELD 42%

RX(13) RCT AC 864234-48-0, AD 106-89-8
RGT AF 1310-58-3 KOH
PRO AH 864234-50-4
SOL 7732-18-5 Water
CON overnight, room temperature

RX(20) RCT AH 864234-50-4, AP 123-75-1
PRO AR 864234-57-1
CON 6 hours, reflux
NTE no solvent

RX(41) OF 57 COMPOSED OF RX(13), RX(22)
RX(41) AC + AD + AS ==> AU



AC

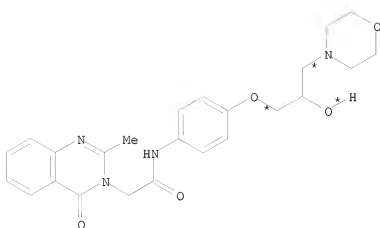


AD



AS

2
STEPS
→

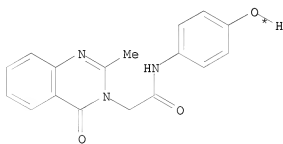


AU
YIELD 20%

RX(13) RCT AC 864234-48-0, AD 106-89-8
RGT AF 1310-58-3 KOH
PRO AH 864234-50-4
SOL 7732-18-5 Water
CON overnight, room temperature

RX(22) RCT AH 864234-50-4, AS 110-91-8
PRO AU 864234-59-3
CON 6 hours, reflux
NTE no solvent

RX(42) OF 57 COMPOSED OF RX(13), RX(24)
RX(42) AC + AD + AV ==> AX



AC

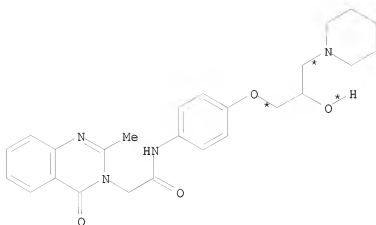


AD



AV

2
STEPS
→



AX

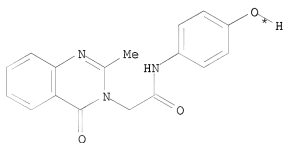
YIELD 35%

RX(13) RCT AC 864234-48-0, AD 106-89-8
 RGT AF 1310-58-3 KOH
 PRO AH 864234-50-4
 SOL 7732-18-5 Water
 CON overnight, room temperature

RX(24) RCT AH 864234-50-4, AV 110-89-4
 PRO AX 864234-61-7
 CON 6 hours, reflux
 NTE no solvent

RX(43) OF 57 COMPOSED OF RX(13), RX(25)

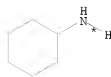
RX(43) AC + AD + AY ==> AZ



AC

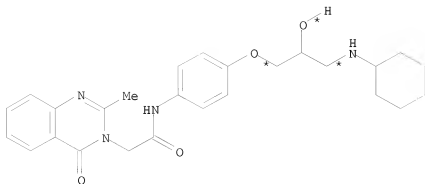


AD



AY

2
 STEPS
 →



AZ

YIELD 32%

RX(13) RCT AC 864234-48-0, AD 106-89-8
 RGT AF 1310-58-3 KOH
 PRO AH 864234-50-4
 SOL 7732-18-5 Water
 CON overnight, room temperature

RX(25) RCT AH 864234-50-4, AY 108-91-8
 PRO AZ 864234-62-8
 CON 6 hours, reflux
 NTE no solvent

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 47 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 143:211923 CASREACT

TITLE: Preparation of fused-ring 4-oxopyrimidine derivatives as histamine H3 receptor antagonists or inverse agonists

INVENTOR(S): Nagase, Tsuyoshi; Sato, Nagaaki; Kanatani, Akio; Tokita, Shigeru

PATENT ASSIGNEE(S): Banyu Pharmaceutical Co., Ltd., Japan

SOURCE: U.S. Pat. Appl. Publ., 84 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050182045	A1	20050818	US 2005-58444	20050214
AU 2005212092	A1	20050825	AU 2005-212092	20050214
CA 2555824	A1	20050825	CA 2005-2555824	20050214
WO 2005077905	A1	20050825	WO 2005-JP2664	20050214

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

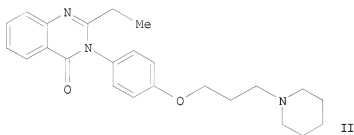
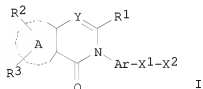
GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1717230 A1 20061102 EP 2005-710446 20050214
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR, IS
 CN 1918128 A 20070221 CN 2005-80004939 20050214
 BR 2005007629 A 20070703 BR 2005-7629 20050214
 JP 4102939 B2 20080618 JP 2005-518071 20050214
 MX 2006009244 A 20061110 MX 2006-9244 20060811
 NO 2006004089 A 20061106 NO 2006-4089 20060912
 IN 2006DN05284 A 20070803 IN 2006-DN5284 20060913
 JP 2008156358 A 20080710 JP 2007-335972 20071227
 JP 2004-37190 JP 2004-37190 20040213
 JP 2005-518071 JP 2005-518071 20050214
 WO 2005-JP2664 WO 2005-JP2664 20050214

PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 143:211923

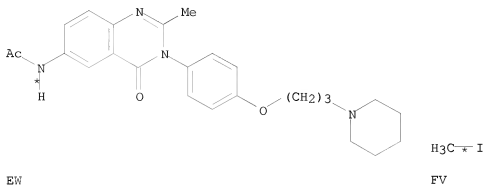
GI



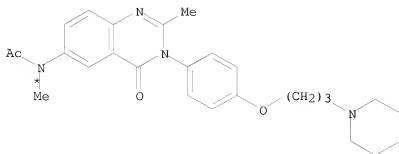
AB The present invention provides fused-ring 4-oxopyrimidines (shown as I; variables defined below; e.g. 2-ethyl-3-[4-(3-(1-piperidinyl)propoxy)phenyl]-4(3H)-quinazolinone (shown as II)) or pharmaceutically acceptable salts thereof, which, having histamine H3 receptor antagonist or inverse agonist activity, are useful in the prophylaxis or therapy of metabolic diseases, circulatory diseases, or nervous system diseases. For I: e.g. Ar is a divalent group formed by eliminating two H atoms from benzene; X1 = N, S, or O; R1 is a 5- to 6-membered heteroaryl group; Ring A is a 5- to 6-membered heteroaryl ring; R2 and R3 are amino or alkylamino groups; Y = CH or N; and X2 = -(CH2)nNR4R5 (R4 and R5 are lower alkyl groups, and n = 2-4). Although the methods of preparation are not claimed, .apprx.275 example preps. are

included. For example, II was prepared in 4 steps (98, 66, 82 and 47 %) starting from anthranilic acid and propionic anhydride and involving intermediates 2-ethyl-4H-3,1-benzoxazin-4-one, 2-ethyl-3-(4-hydroxyphenyl)-4(3H)-quinazolinone, and 2-ethyl-3-[4-(3-chloropropoxy)phenyl]-4(3H)-quinazolinone. Pharmacol. results are provided for II for the following tests: histamine analog coupling inhibition, antagonism of drinking behavior induced by R- α -methylhistamine (a histamine H3 receptor selective agonist), in vitro kinetics, and brain/cerebrospinal fluid activity.

RX(97) OF 861 ...EW + FV ==> FW



(97)
→



FW

RX(97) RCT EW 862309-53-3

STAGE(1)

RGT BM 7646-69-7 NaH

STAGE(2)

RCT FV 74-88-4

SOL 109-99-9 THF, 110-86-1 Pyridine

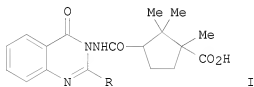
CON SUBSTAGE(1) cooled

SUBSTAGE(2) cooled

SUBSTAGE(3) overnight, room temperature

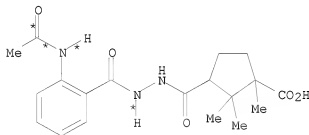
PRO FW 862309-89-5

L3 ANSWER 48 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 143:172829 CASREACT
 TITLE: Synthesis of (±)-1,2,2-trimethyl-1,3-cyclopentanedicarboxylic acid derivatives with a 4(3H)-quinazolinone fragment
 AUTHOR(S): Gritsenko, I. S.; Tsapko, Ye. A.
 CORPORATE SOURCE: Nats. Farm. Univ., Kharkov, 61146, Ukraine
 SOURCE: Zhurnal Organichnoi ta Farmatsevtichnoi Khimii (2005), 3(1), 12-16
 CODEN: ZOFKAM
 PUBLISHER: Natsional'nii Farmatsevtichnii Universitet
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



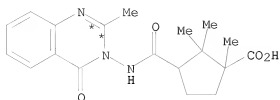
AB The hydrazide of anthranilic acid has been acylated by 1,2,2-trimethylcyclopentanedicarboxylic acid anhydride. The product of the reaction was cyclized to the title compds. (I; R = Me, Et, Pr, CC13).

RX(14) OF 64 ...G ==> N...



(14) →

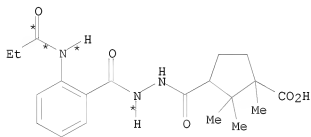
10/ 562,112



N
YIELD 83%

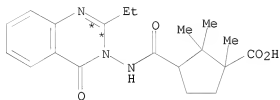
RX(14) RCT G 860479-66-9
 RGT V 68-12-2 DMF
 PRO N 860479-70-5
 SOL 1330-20-7 Xylene
 CON 15 - 20 minutes, reflux
 NTE regioselective, alternative preparation shown, brombenzene/agent
 gave similar results

RX(15) OF 64 ...I ==> P...



I

(15)
→



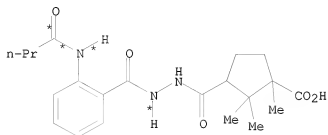
P
YIELD 78%

RX(15) RCT I 860479-67-0
 RGT V 68-12-2 DMF
 PRO P 860479-71-6
 SOL 1330-20-7 Xylene
 CON 15 - 20 minutes, reflux
 NTE regioselective, alternative preparation shown, brombenzene/agent

10/ 562,112

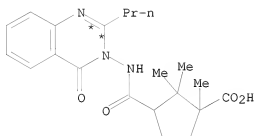
gave similar results

RX(16) OF 64 ...K ==> Q...



K

(16)
→

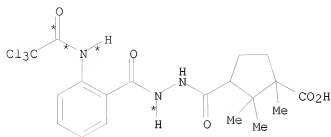


Q

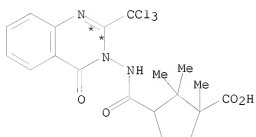
YIELD 69%

RX(16) RCT K 860479-68-1
 RGT V 68-12-2 DMF
 PRO Q 860479-72-7
 SOL 1330-20-7 Xylene
 CON SUBSTAGE(1) 15 - 20 minutes, reflux
 SUBSTAGE(2) cooled
 NTE regioselective, alternative preparation shown, brombenzene/agent
 gave similar results

RX(17) OF 64 ...M ==> R



M

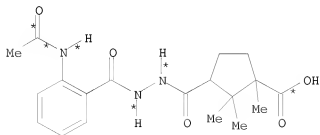
(17) \longrightarrow 

R

YIELD 76%

RX(17) RCT M 860479-69-2
 RGT V 68-12-2 DMF
 PRO R 860479-73-8
 SOL 1330-20-7 Xylene
 CON 15 - 20 minutes, reflux
 NTE regioselective, alternative preparation shown, brombenzene/agent
 gave similar results

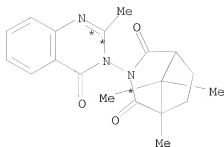
RX(19) OF 64 ...G ==> S



G

(19) \longrightarrow

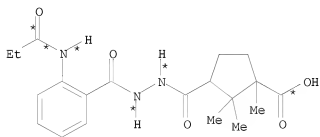
10/ 562,112



S
YIELD 88%

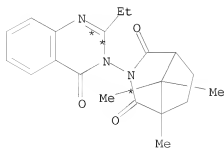
RX(19) RCT G 860479-66-9
 PRO S 860479-74-9
 CON 45 minutes, 220 - 230 deg C
 NTE regioselective, thermal, alternative preparation shown, no solvent

RX(21) OF 64 ...I ==> T



I

(21) \longrightarrow



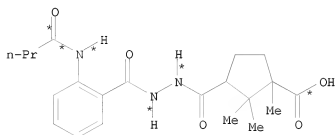
T
YIELD 78%

RX(21) RCT I 860479-67-0
 PRO T 860479-75-0

10/ 562,112

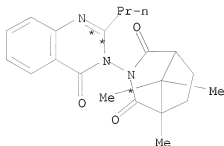
CON 45 minutes, 220 - 230 deg C
NTE regioselective, thermal, alternative preparation shown, no solvent

RX(23) OF 64 ...K ==> U



K

(23) →

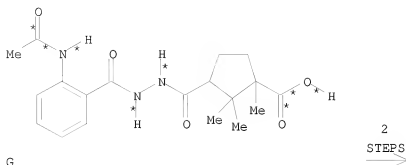


U

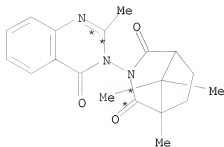
YIELD 76%

RX(23) RCT K 860479-68-1
PRO U 860479-76-1
CON 45 minutes, 220 - 230 deg C
NTE regioselective, thermal, alternative preparation shown, no solvent

RX(44) OF 64 COMPOSED OF RX(14), RX(18)
RX(44) G ==> S



G



S

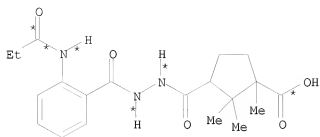
YIELD 89%

RX(14) RCT G 860479-66-9
 RGT V 68-12-2 DMF
 PRO N 860479-70-5
 SOL 1330-20-7 Xylene
 CON 15 - 20 minutes, reflux
 NTE regioselective, alternative preparation shown, brombenzene/agent gave similar results

RX(18) RCT N 860479-70-5
 RGT X 108-24-7 Ac2O
 PRO S 860479-74-9
 SOL 64-19-7 AcOH
 CON 40 minutes, heated
 NTE regioselective, alternative preparation shown

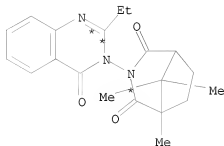
RX(46) OF 64 COMPOSED OF RX(15), RX(20)

RX(46) I ==> T



I

2
STEPS
→



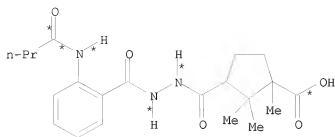
T

RX(15) RCT I 860479-67-0
 RGT V 68-12-2 DMF
 PRO P 860479-71-6
 SOL 1330-20-7 Xylene
 CON 15 - 20 minutes, reflux
 NTE regioselective, alternative preparation shown, brombenzene/agent
 gave similar results

RX(20) RCT P 860479-71-6
 RGT X 108-24-7 Ac2O
 PRO T 860479-75-0
 SOL 64-19-7 AcOH
 CON 40 minutes, heated
 NTE regioselective, alternative preparation shown

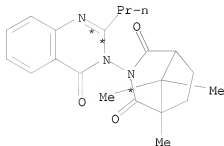
RX(48) OF 64 COMPOSED OF RX(16), RX(22)

RX(48) K ==> U



K

2
STEPS
→



U

RX(16) RCT K 860479-68-1
 RGT V 68-12-2 DMF
 PRO Q 860479-72-7
 SOL 1330-20-7 Xylene
 CON SUBSTAGE(1) 15 - 20 minutes, reflux
 SUBSTAGE(2) cooled
 NTE regioselective, alternative preparation shown, brombenzene/agent gave similar results

RX(22) RCT Q 860479-72-7
 RGT X 108-24-7 Ac2O
 PRO U 860479-76-1
 SOL 64-19-7 AcOH
 CON 40 minutes, heated
 NTE regioselective, alternative preparation shown

L3 ANSWER 49 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

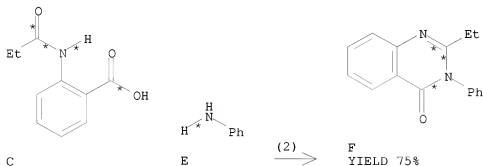
ACCESSION NUMBER: 143:153337 CASREACT

TITLE: Synthesis and structure-activity relationship of
 3-phenyl-3H-quinazolin-4-one derivatives as CXCR3
 chemokine receptor antagonists

AUTHOR(S): Storelli, Stefania; Verdijk, Pauline; Verzijl, Dennis;
 Timmerman, Henk; van de Stolpe, Andrea C.; Tensen,
 Cornelis P.; Smit, Martine J.; De Esch, Iwan J. P.;

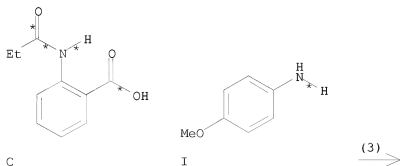
CORPORATE SOURCE: Leurs, Rob
 Leiden/Amsterdam Center for Drug Research (LACDR),
 Division of Medicinal Chemistry, Faculty of Sciences,
 Vrije Universiteit Amsterdam, Amsterdam, 1081 HV,
 Neth.
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2005),
 15(11), 2910-2913
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A series of 3-phenyl-3H-quinazolin-4-ones have been synthesized and tested
 for affinity and activity at the chemokine CXCR3 receptor. The most
 potent compound has been evaluated using radioligand binding and calcium
 mobilization assays and is considered a useful tool for further
 characterization of the CXCR3 receptor.

RX(2) OF 173 ...C + E ==> F...

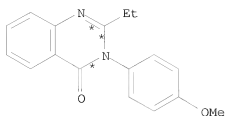


RX(2) RCT C 19165-26-5, E 62-53-3
 RGT G 7719-12-2 PC13
 PRO F 5260-41-3
 SOL 108-88-3 PhMe

RX(3) OF 173 ...C + I ==> J...



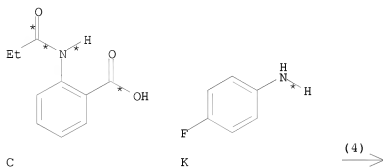
10/ 562,112



J
YIELD 75%

RX(3) RCT C 19165-26-5, I 104-94-9
RGT G 7719-12-2 PC13
PRO J 50498-62-9
SOL 108-88-3 PhMe

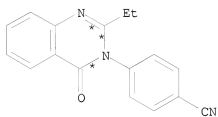
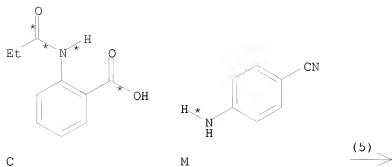
RX(4) OF 173 ...C + K ==> L...



L
YIELD 75%

RX(4) RCT C 19165-26-5, K 371-40-4
RGT G 7719-12-2 PC13
PRO L 329190-48-9
SOL 108-88-3 PhMe

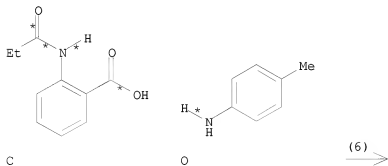
RX(5) OF 173 ...C + M ==> N...



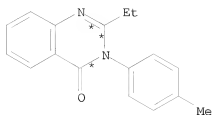
YIELD 75%

RX(5) RCT C 19165-26-5, M 873-74-5
 RGT G 7719-12-2 FC13
 PRO N 860002-79-5
 SOL 108-88-3 PhMe

RX(6) OF 173 ...C + O ==> P...



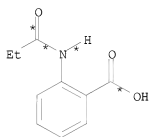
10/ 562,112



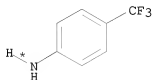
P
YIELD 75%

RX(6) RCT C 19165-26-5, O 106-49-0
 RGT G 7719-12-2 PC13
 PRO P 50498-61-8
 SOL 108-88-3 PhMe

RX(7) OF 173 ...C + Q ==> R...

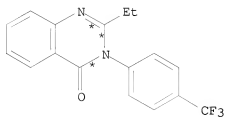


C



Q

(7) >

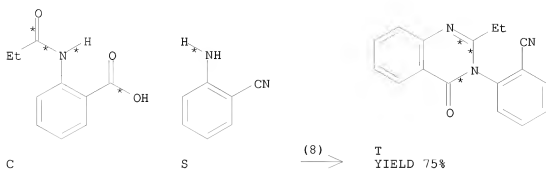


R
YIELD 75%

RX(7) RCT C 19165-26-5, Q 455-14-1
 RGT G 7719-12-2 PC13
 PRO R 860002-80-8
 SOL 108-88-3 PhMe

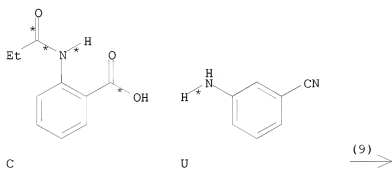
10/ 562,112

RX(8) OF 173 ...C + S ==> T...



RX(8) RCT C 19165-26-5, S 1885-29-6
RGT G 7719-12-2 PC13
PRO T 860002-81-9
SOL 108-88-3 PhMe

RX(9) OF 173 ...C + U ==> V...



V
YIELD 75%

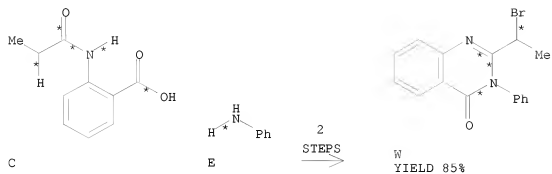
RX(9) RCT C 19165-26-5, U 2237-30-1
RGT G 7719-12-2 PC13
PRO V 860002-82-0

10/ 562,112

SOL 108-88-3 PhMe

RX(49) OF 173 COMPOSED OF RX(2), RX(10)

RX(49) C + E ==> W



RX(2) RCT C 19165-26-5, E 62-53-3

RGT G 7719-12-2 PC13

PRO F 5260-41-3

SOL 108-88-3 PhMe

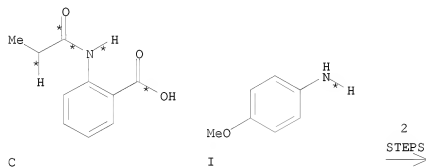
RX(10) RCT F 5260-41-3

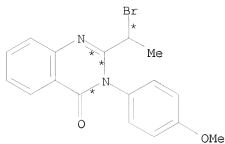
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br₂

PRO W 860002-83-1

RX(50) OF 173 COMPOSED OF RX(3), RX(11)

RX(50) C + I ==> AA





AA

YIELD 85%

RX(3) RCT C 19165-26-5, I 104-94-9

RGT G 7719-12-2 PC13

PRO J 50498-62-9

SOL 108-88-3 PhMe

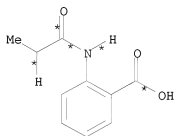
RX(11) RCT J 50498-62-9

RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2

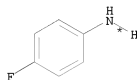
PRO AA 473721-15-2

RX(51) OF 173 COMPOSED OF RX(4), RX(12)

RX(51) C + K ==> AB

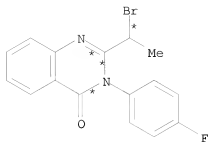


C



K

2
STEPS
→



AB

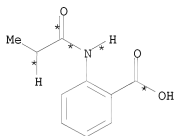
YIELD 85%

RX(4) RCT C 19165-26-5, K 371-40-4
 RGT G 7719-12-2 PC13
 PRO L 329190-48-9
 SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AB 329190-49-0

RX(52) OF 173 COMPOSED OF RX(5), RX(13)

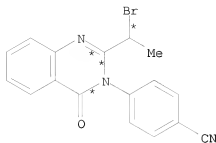
RX(52) C + M ==> AC



C

M

2
 STEPS
 →



AC

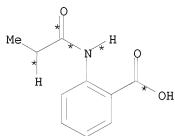
YIELD 85%

RX(5) RCT C 19165-26-5, M 873-74-5
 RGT G 7719-12-2 PC13
 PRO N 860002-79-5
 SOL 108-88-3 PhMe

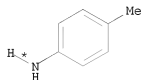
RX(13) RCT N 860002-79-5
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AC 860002-84-2

RX(53) OF 173 COMPOSED OF RX(6), RX(14)

RX(53) C + O ==> AD

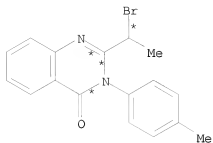


C



O

2
 STEPS
 →



AD

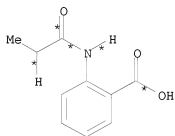
YIELD 85%

RX(6) RCT C 19165-26-5, O 106-49-0
 RGT G 7719-12-2 PC13
 PRO P 50498-61-8
 SOL 108-88-3 PhMe

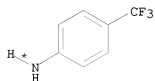
RX(14) RCT P 50498-61-8
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AD 860002-85-3

RX(54) OF 173 COMPOSED OF RX(7), RX(15)

RX(54) C + Q ==> AE

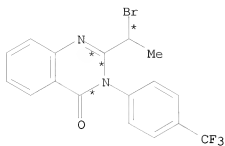


C



Q

2
 STEPS
 →

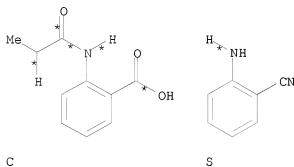


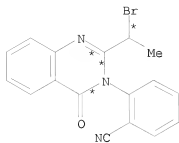
AE
YIELD 85%

RX(7) RCT C 19165-26-5, Q 455-14-1
RGT G 7719-12-2 PC13
PRO R 860002-80-8
SOL 108-88-3 PhMe

RX(15) RCT R 860002-80-8
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
PRO AE 860002-86-4

RX(55) OF 173 COMPOSED OF RX(8), RX(16)
RX(55) C + S ==> AF





AF

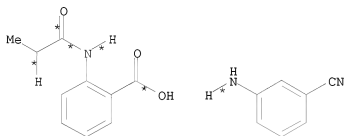
YIELD 85%

RX(8) RCT C 19165-26-5, S 1885-29-6
 RGT G 7719-12-2 PC13
 PRO T 860002-81-9
 SOL 108-88-3 PhMe

RX(16) RCT T 860002-81-9
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AF 860002-87-5

RX(56) OF 173 COMPOSED OF RX(9), RX(17)

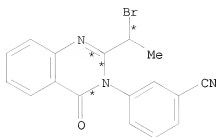
RX(56) C + U ==> AG



C

U

2
 STEPS
 →



AG

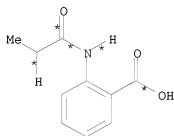
YIELD 85%

RX(9) RCT C 19165-26-5, U 2237-30-1
 RGT G 7719-12-2 PC13
 PRO V 860002-82-0
 SOL 108-88-3 PhMe

RX(17) RCT V 860002-82-0
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AG 860002-88-6

RX(89) OF 173 COMPOSED OF RX(2), RX(10), RX(18)

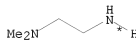
RX(89) C + E + AH ==> AI



C

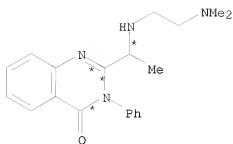


E



AH

3
 STEPS
 →



AI

YIELD 65%

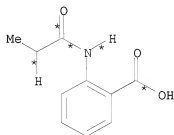
RX(2) RCT C 19165-26-5, E 62-53-3
 RGT G 7719-12-2 PC13
 PRO F 5260-41-3
 SOL 108-88-3 PhMe

RX(10) RCT F 5260-41-3
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO W 860002-83-1

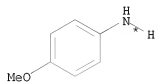
RX(18) RCT W 860002-83-1, AH 108-00-9
 PRO AI 860002-89-7
 SOL 64-17-5 EtOH
 CON reflux

RX(91) OF 173 COMPOSED OF RX(3), RX(11), RX(19)

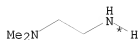
RX(91) C + I + AH ==> AK



C

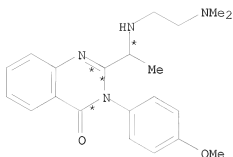


I



AH

3
 STEPS
 →



AK

YIELD 65%

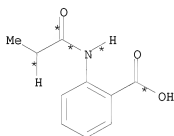
RX(3) RCT C 19165-26-5, I 104-94-9
 RGT G 7719-12-2 PC13
 PRO J 50498-62-9
 SOL 108-88-3 PhMe

RX(11) RCT J 50498-62-9
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AA 473721-15-2

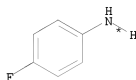
RX(19) RCT AA 473721-15-2, AH 108-00-9
 PRO AK 473721-16-3
 SOL 64-17-5 EtOH
 CON reflux

RX(93) OF 173 COMPOSED OF RX(4), RX(12), RX(20)

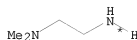
RX(93) C + K + AH ==> AL



C

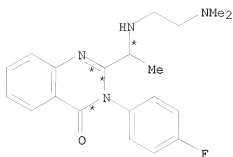


K



AH

3
 STEPS
 →



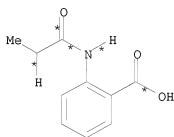
AL
YIELD 65%

RX(4) RCT C 19165-26-5, K 371-40-4
RGT G 7719-12-2 PC13
PRO L 329190-48-9
SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
PRO AB 329190-49-0

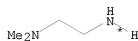
RX(20) RCT AB 329190-49-0, AH 108-00-9
PRO AL 329190-50-3
SOL 64-17-5 EtOH
CON reflux

RX(95) OF 173 COMPOSED OF RX(5), RX(13), RX(21)
RX(95) C + M + AH ==> AM



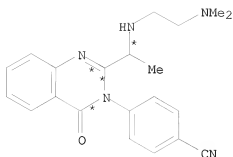
C

M



AH

3
STEPS
→



AM

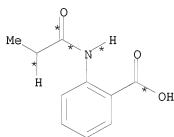
YIELD 65%

RX(5) RCT C 19165-26-5, M 873-74-5
 RGT G 7719-12-2 PC13
 PRO N 860002-79-5
 SOL 108-88-3 PhMe

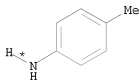
RX(13) RCT N 860002-79-5
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AC 860002-84-2

RX(21) RCT AC 860002-84-2, AH 108-00-9
 PRO AM 860002-90-0
 SOL 64-17-5 EtOH
 CON reflux

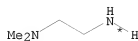
RX(97) OF 173 COMPOSED OF RX(6), RX(14), RX(22)
 RX(97) C + O + AH ==> AN



C



O

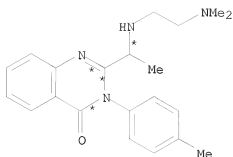


AH

3

STEPS





AN

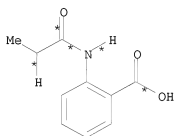
YIELD 65%

RX(6) RCT C 19165-26-5, O 106-49-0
 RGT G 7719-12-2 PC13
 PRO P 50498-61-8
 SOL 108-88-3 PhMe

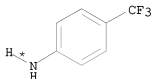
RX(14) RCT P 50498-61-8
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AD 860002-85-3

RX(22) RCT AD 860002-85-3, AH 108-00-9
 PRO AN 854622-82-5
 SOL 64-17-5 EtOH
 CON reflux

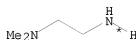
RX(99) OF 173 COMPOSED OF RX(7), RX(15), RX(23)
 RX(99) C + Q + AH ==> AO



C



Q

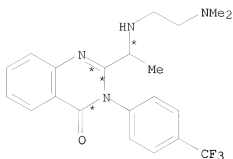


AH

3

STEPS





AO

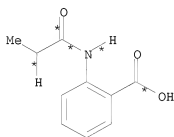
YIELD 65%

RX(7) RCT C 19165-26-5, Q 455-14-1
 RGT G 7719-12-2 PC13
 PRO R 860002-80-8
 SOL 108-88-3 PhMe

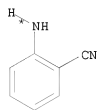
RX(15) RCT R 860002-80-8
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AE 860002-86-4

RX(23) RCT AE 860002-86-4, AH 108-00-9
 PRO AO 860002-91-1
 SOL 64-17-5 EtOH
 CON reflux

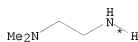
RX(101) OF 173 COMPOSED OF RX(8), RX(16), RX(24)
 RX(101) C + S + AH ==> AP



C

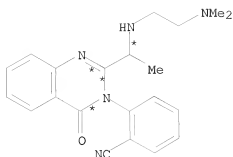


S



AH

3
 STEPS
 →



AP

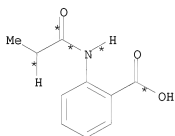
YIELD 65%

RX(8) RCT C 19165-26-5, S 1885-29-6
 RGT G 7719-12-2 PC13
 PRO T 860002-81-9
 SOL 108-88-3 PhMe

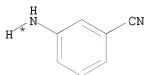
RX(16) RCT T 860002-81-9
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AF 860002-87-5

RX(24) RCT AF 860002-87-5, AH 108-00-9
 PRO AP 860002-92-2
 SOL 64-17-5 EtOH
 CON reflux

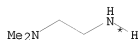
RX(103) OF 173 COMPOSED OF RX(9), RX(17), RX(25)
 RX(103) C + U + AH ==> AQ



C

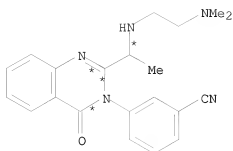


U



AH

3
 STEPS
 →



AQ

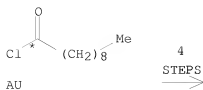
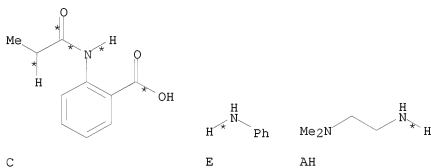
YIELD 65%

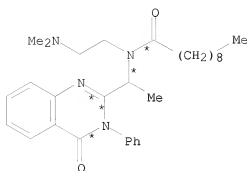
RX(9) RCT C 19165-26-5, U 2237-30-1
 RGT G 7719-12-2 PC13
 PRO V 860002-82-0
 SOL 108-88-3 PhMe

RX(17) RCT V 860002-82-0
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AG 860002-88-6

RX(25) RCT AG 860002-88-6, AH 108-00-9
 PRO AQ 860002-93-3
 SOL 64-17-5 EtOH
 CON reflux

RX(106) OF 173 COMPOSED OF RX(2), RX(10), RX(18), RX(27)
 RX(106) C + E + AH + AU ==> AV





AV

YIELD 55%

RX(2) RCT C 19165-26-5, E 62-53-3
 RGT G 7719-12-2 PC13
 PRO F 5260-41-3
 SOL 108-88-3 PhMe

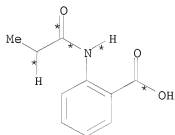
RX(10) RCT F 5260-41-3
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO W 860002-83-1

RX(18) RCT W 860002-83-1, AH 108-00-9
 PRO AI 860002-89-7
 SOL 64-17-5 EtOH
 CON reflux

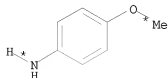
RX(27) RCT AI 860002-89-7, AU 112-13-0
 RGT AW 121-44-8 Et3N
 PRO AV 334516-31-3
 SOL 123-91-1 Dioxane

RX(109) OF 173 COMPOSED OF RX(3), RX(11), RX(19), RX(26)

RX(109) C + I + AH ==> AR



C



I



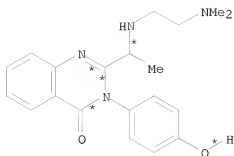
AH

4

STEPS



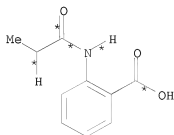
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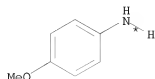
AR
YIELD 15%

RX(3)	RCT	C 19165-26-5, I 104-94-9
	RGT	G 7719-12-2 PC13
	PRO	J 50498-62-9
	SOL	108-88-3 PhMe
RX(11)	RCT	J 50498-62-9
	RGT	X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
	PRO	AA 473721-15-2
RX(19)	RCT	AA 473721-15-2, AH 108-00-9
	PRO	AK 473721-16-3
	SOL	64-17-5 EtOH
	CON	reflux
RX(26)	RCT	AK 473721-16-3
	RGT	AS 10294-33-4 BBr3
	PRO	AR 860002-94-4
	SOL	67-56-1 MeOH

RX(110) OF 173 COMPOSED OF RX(3), RX(11), RX(19), RX(28)
RX(110) C + I + AH + AU ==> AY



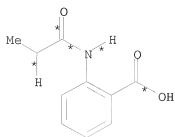
C



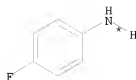
I



AH



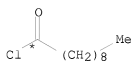
C



K

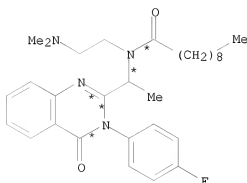


AH



AU

4
STEPS



AZ
YIELD 55%

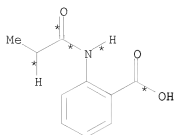
RX(4) RCT C 19165-26-5, K 371-40-4
 RGT G 7719-12-2 PC13
 PRO L 329190-48-9
 SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AB 329190-49-0

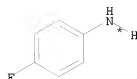
RX(20) RCT AB 329190-49-0, AH 108-00-9
 PRO AL 329190-50-3
 SOL 64-17-5 EtOH
 CON reflux

RX(29) RCT AL 329190-50-3, AU 112-13-0
 RGT AW 121-44-8 Et3N
 PRO AZ 329190-29-6
 SOL 123-91-1 Dioxane

RX(117) OF 173 COMPOSED OF RX(4), RX(12), RX(20), RX(35)
 RX(117) C + K + AH + AY + BF ==> BG + BH



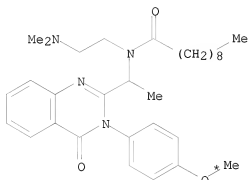
C



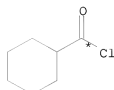
K



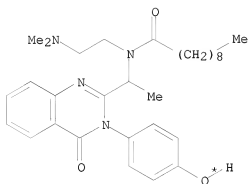
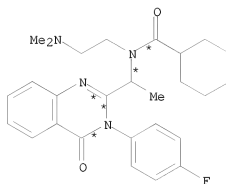
AH



AY



BF

4
STEPS
→BG
YIELD 15%BH
YIELD 55%

RX(4) RCT C 19165-26-5, K 371-40-4
RGT G 7719-12-2 PC13
PRO L 329190-48-9
SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9

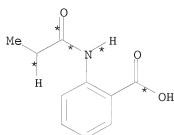
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RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
PRO AB 329190-49-0

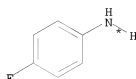
RX(20) RCT AB 329190-49-0, AH 108-00-9
PRO AL 329190-50-3
SOL 64-17-5 EtOH
CON reflux

RX(35) RCT AL 329190-50-3, AY 329190-30-9, BF 2719-27-9
RGT AW 121-44-8 Et3N, AS 10294-33-4 BBr3
PRO BG 860002-99-9, BH 860003-00-5
SOL 67-56-1 MeOH, 123-91-1 Dioxane

RX(118) OF 173 COMPOSED OF RX(4), RX(12), RX(20), RX(36)
RX(118) C + K + AH + BF ==> BH



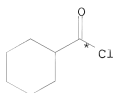
C



K

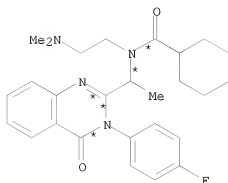


AH



BF

4
STEPS
→



BH
YIELD 55%

RX(4) RCT C 19165-26-5, K 371-40-4
RGT G 7719-12-2 PC13
PRO L 329190-48-9
SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2

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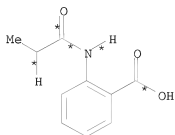
PRO AB 329190-49-0

RX(20) RCT AB 329190-49-0, AH 108-00-9
PRO AL 329190-50-3
SOL 64-17-5 EtOH
CON reflux

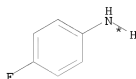
RX(36) RCT AL 329190-50-3, BF 2719-27-9
RGT AW 121-44-8 Et3N
PRO BH 860003-00-5
SOL 123-91-1 Dioxane

RX(119) OF 173 COMPOSED OF RX(4), RX(12), RX(20), RX(38)

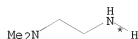
RX(119) C + K + AH + BJ ==> BK



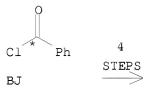
C



K

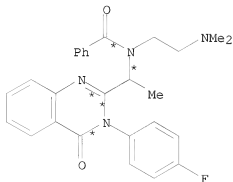


AH



BJ

4
STEPS
→



BK
YIELD 55%

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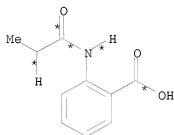
RX(4) RCT C 19165-26-5, K 371-40-4
 RGT G 7719-12-2 PC13
 PRO L 329190-48-9
 SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AB 329190-49-0

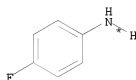
RX(20) RCT AB 329190-49-0, AH 108-00-9
 PRO AL 329190-50-3
 SOL 64-17-5 EtOH
 CON reflux

RX(38) RCT AL 329190-50-3, BJ 98-88-4
 RGT AW 121-44-8 Et3N
 PRO BK 860003-02-7
 SOL 123-91-1 Dioxane

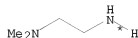
RX(120) OF 173 COMPOSED OF RX(4), RX(12), RX(20), RX(40)
 RX(120) C + K + AH + BM ==> BN



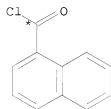
C



K

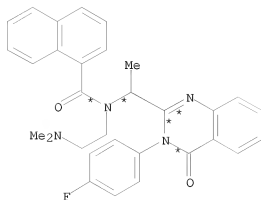


AH



BM

4
 STEPS
 →



BN
 YIELD 55%

RX(4) RCT C 19165-26-5, K 371-40-4

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RGT G 7719-12-2 PC13
 PRO L 329190-48-9
 SOL 108-88-3 PhMe

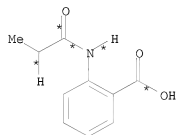
RX(12) RCT L 329190-48-9
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AB 329190-49-0

RX(20) RCT AB 329190-49-0, AH 108-00-9
 PRO AL 329190-50-3
 SOL 64-17-5 EtOH
 CON reflux

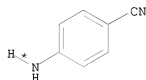
RX(40) RCT AL 329190-50-3, BM 879-18-5
 RGT AW 121-44-8 Et3N
 PRO BN 334904-56-2
 SOL 123-91-1 Dioxane

RX(124) OF 173 COMPOSED OF RX(5), RX(13), RX(21), RX(30)

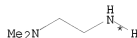
RX(124) C + M + AH + AU ==> BA



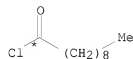
C



M

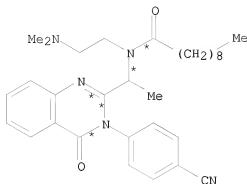


AH



AU

4
 STEPS
 →



BA

YIELD 55%

RX(5) RCT C 19165-26-5, M 873-74-5
 RGT G 7719-12-2 PC13
 PRO N 860002-79-5
 SOL 108-88-3 PhMe

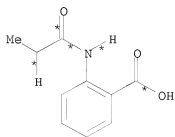
RX(13) RCT N 860002-79-5
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AC 860002-84-2

RX(21) RCT AC 860002-84-2, AH 108-00-9
 PRO AM 860002-90-0
 SOL 64-17-5 EtOH
 CON reflux

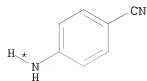
RX(30) RCT AM 860002-90-0, AU 112-13-0
 RGT AW 121-44-8 Et3N
 PRO BA 860002-95-5
 SOL 123-91-1 Dioxane

RX(125) OF 173 COMPOSED OF RX(5), RX(13), RX(21), RX(37)

RX(125) C + M + AH + BF ==> BI



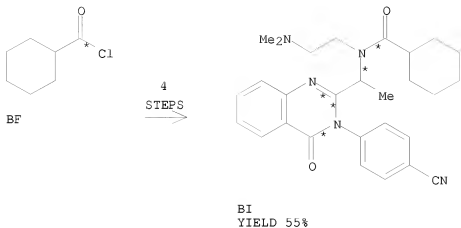
C



M



AH



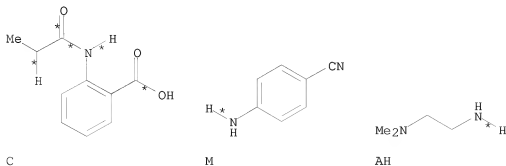
RX(5) RCT C 19165-26-5, M 873-74-5
 RGT G 7719-12-2 PCl3
 PRO N 860002-79-5
 SOL 108-88-3 PhMe

RX(13) RCT N 860002-79-5
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AC 860002-84-2

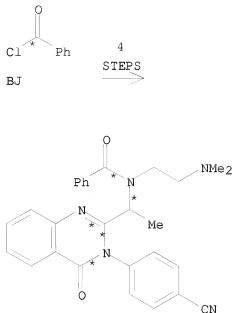
RX(21) RCT AC 860002-84-2, AH 108-00-9
 PRO AM 860002-90-0
 SOL 64-17-5 EtOH
 CON reflux

RX(37) RCT AM 860002-90-0, BF 2719-27-9
 RGT AW 121-44-8 Et3N
 PRO BI 860003-01-6
 SOL 123-91-1 Dioxane

RX(126) OF 173 COMPOSED OF RX(5), RX(13), RX(21), RX(39)
 RX(126) C + M + AH + BJ ==> BL



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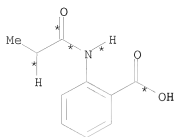
RX(5) RCT C 19165-26-5, M 873-74-5
 RGT G 7719-12-2 PC13
 PRO N 860002-79-5
 SOL 108-88-3 PhMe

RX(13) RCT N 860002-79-5
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AC 860002-84-2

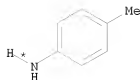
RX(21) RCT AC 860002-84-2, AH 108-00-9
 PRO AM 860002-90-0
 SOL 64-17-5 EtOH
 CON reflux

RX(39) RCT AM 860002-90-0, BJ 98-88-4
 RGT AW 121-44-8 Et3N
 PRO BL 860003-03-8
 SOL 123-91-1 Dioxane

RX(128) OF 173 COMPOSED OF RX(6), RX(14), RX(22), RX(31)
 RX(128) C + O + AH + AU ==> BB



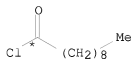
C



O

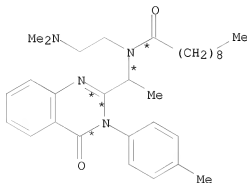


AH



AU

4
STEPS



BB
YIELD 55%

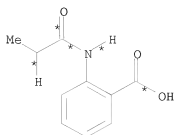
RX(6) RCT C 19165-26-5, O 106-49-0
RGT G 7719-12-2 PC13
PRO P 50498-61-8
SOL 108-88-3 PhMe

RX(14) RCT P 50498-61-8
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
PRO AD 860002-85-3

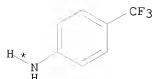
RX(22) RCT AD 860002-85-3, AH 108-00-9
PRO AN 854622-82-5
SOL 64-17-5 EtOH
CON reflux

RX(31) RCT AN 854622-82-5, AU 112-13-0
RGT AW 121-44-8 Et3N
PRO BB 334801-64-8
SOL 123-91-1 Dioxane

RX(130) OF 173 COMPOSED OF RX(7), RX(15), RX(23), RX(32)
RX(130) C + Q + AH + AU ==> BC



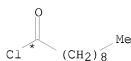
C



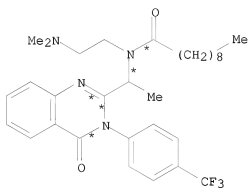
Q



AH



AU

4
STEPS
→

BC

YIELD 55%

RX(7) RCT C 19165-26-5, Q 455-14-1
 RGT G 7719-12-2 PC13
 PRO R 860002-80-8
 SOL 108-88-3 PhMe

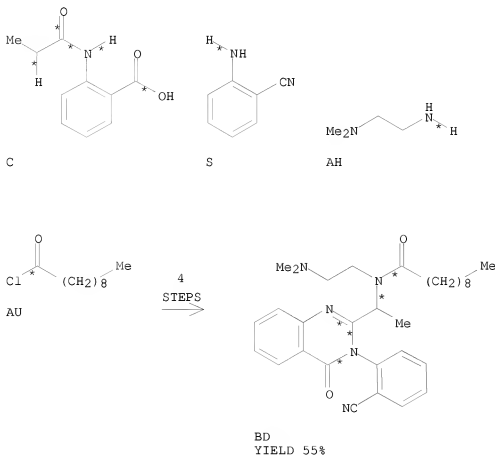
RX(15) RCT R 860002-80-8
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AE 860002-86-4

RX(23) RCT AE 860002-86-4, AH 108-00-9
 PRO AO 860002-91-1
 SOL 64-17-5 EtOH
 CON reflux

RX(32) RCT AO 860002-91-1, AU 112-13-0
 RGT AW 121-44-8 Et3N
 PRO BC 860002-96-6

SOL 123-91-1 Dioxane

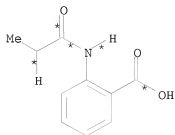
RX(132) OF 173 COMPOSED OF RX(8), RX(16), RX(24), RX(33)
 RX(132) C + S + AH + AU ==> BD



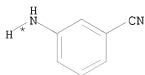
RX(8)	RCT C 19165-26-5, S 1885-29-6
	RGT G 7719-12-2 PC13
	PRO T 860002-81-9
	SOL 108-88-3 PhMe
RX(16)	RCT T 860002-81-9
	RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
	PRO AF 860002-87-5
RX(24)	RCT AF 860002-87-5, AH 108-00-9
	PRO AP 860002-92-2
	SOL 64-17-5 EtOH
	CON reflux
RX(33)	RCT AP 860002-92-2, AU 112-13-0
	RGT AW 121-44-8 Et3N
	PRO BD 860002-97-7
	SOL 123-91-1 Dioxane

RX(134) OF 173 COMPOSED OF RX(9), RX(17), RX(25), RX(34)

RX(134) C + U + AH + AU ==> BE



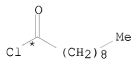
C



U

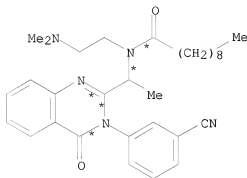


AH



AU

4
STEPS
→



BE

YIELD 55%

RX(9) RCT C 19165-26-5, U 2237-30-1

RGT G 7719-12-2 PC13

PRO V 860002-82-0

SOL 108-88-3 PhMe

RX(17) RCT V 860002-82-0

RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2

PRO AG 860002-88-6

RX(25) RCT AG 860002-88-6, AH 108-00-9

PRO AQ 860002-93-3

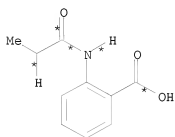
SOL 64-17-5 EtOH

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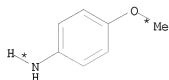
CON reflux

RX(34) RCT AQ 860002-93-3, AU 112-13-0
 RGT AW 121-44-8 Et3N
 PRO BE 860002-98-8
 SOL 123-91-1 Dioxane

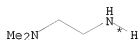
RX(155) OF 173 COMPOSED OF RX(3), RX(11), RX(19), RX(28), RX(35)
 RX(155) C + I + AH + AU + AL + BF ==> BG +
 BH



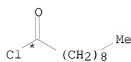
C



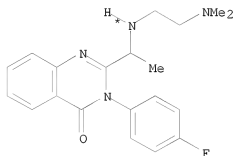
I



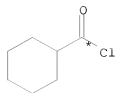
AH



AU

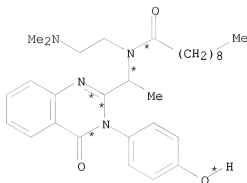


AL

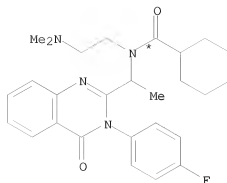


BF

5
 STEPS
 →



BG
YIELD 15%



BH
YIELD 55%

```

RX(3)    RCT  C 19165-26-5, I 104-94-9
          RGT  G 7719-12-2 PC13
          PRO  J 50498-62-9
          SOL  108-88-3 PhMe

RX(11)   RCT  J 50498-62-9
          RGT  X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
          PRO  AA 473721-15-2

RX(19)   RCT  AA 473721-15-2, AH 108-00-9
          PRO  AK 473721-16-3
          SOL  64-17-5 EtOH
          CON  reflux

RX(28)   RCT  AK 473721-16-3, AU 112-13-0
          RGT  AW 121-44-8 Et3N
          PRO  AY 329190-30-9
          SOL  123-91-1 Dioxane

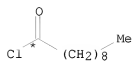
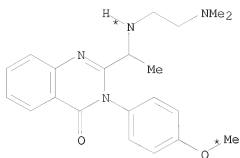
RX(35)   RCT  AL 329190-50-3, AY 329190-30-9, BF 2719-27-9
          RGT  AW 121-44-8 Et3N, AS 10294-33-4 BBr3
          PRO  BG 860002-99-9, BH 860003-00-5
          SOL  67-56-1 MeOH, 123-91-1 Dioxane

```

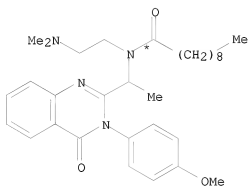
```

RX(157) OF 173 COMPOSED OF REACTION SEQUENCE RX(28), RX(35)
          AND REACTION SEQUENCE RX(4), RX(12), RX(20), RX(35)
...AK + AU ==> AY...
... C + K + AH + AY + BF ==> BG + BH

```

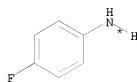
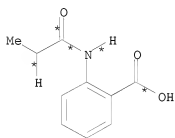


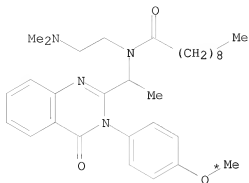
4
STEPS
→



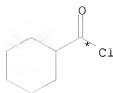
AY

START NEXT REACTION SEQUENCE



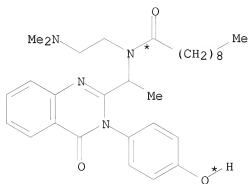


AY

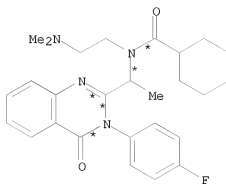


BF

4
STEPS
→



BG
YIELD 15%



BH
YIELD 55%

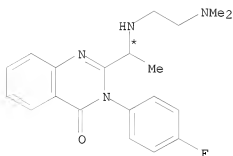
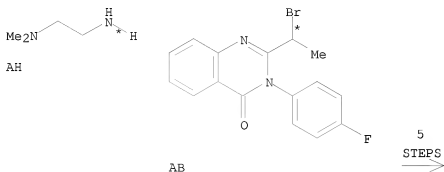
RX(28)	RCT	AK 473721-16-3, AU 112-13-0
	RGT	AW 121-44-8 Et3N
	PRO	AY 329190-30-9
	SOL	123-91-1 Dioxane
RX(4)	RCT	C 19165-26-5, K 371-40-4
	RGT	G 7719-12-2 PC13
	PRO	L 329190-48-9
	SOL	108-88-3 PhMe
RX(12)	RCT	L 329190-48-9
	RGT	X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
	PRO	AB 329190-49-0
RX(20)	RCT	AB 329190-49-0, AH 108-00-9
	PRO	AL 329190-50-3
	SOL	64-17-5 EtOH
	CON	reflux
RX(35)	RCT	AL 329190-50-3, AY 329190-30-9, BF 2719-27-9
	RGT	AW 121-44-8 Et3N, AS 10294-33-4 BBr3

PRO BG 860002-99-9, BH 860003-00-5
 SOL 67-56-1 MeOH, 123-91-1 Dioxane

RX(160) OF 173 COMPOSED OF REACTION SEQUENCE RX(20), RX(35)
 AND REACTION SEQUENCE RX(3), RX(11), RX(19), RX(28), RX(35)

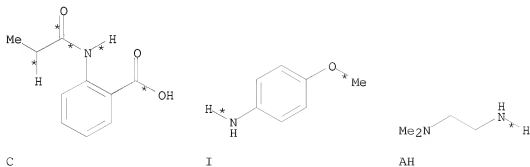
...AB + AH ==> AL...

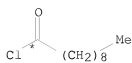
... C + I + AH + AU + AL + BF ==> BG + BH



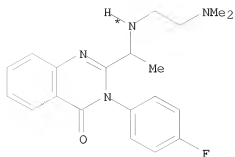
AL

START NEXT REACTION SEQUENCE

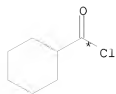




AU

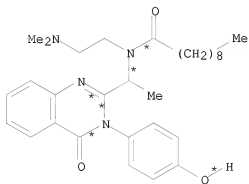


AL



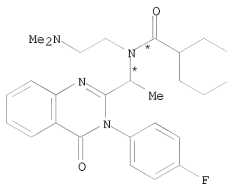
BF

5
STEPS
→



BG

YIELD 15%



BH

YIELD 55%

RX(20) RCT AB 329190-49-0, AH 108-00-9
PRO AL 329190-50-3
SOL 64-17-5 EtOH
CON reflux

RX(3) RCT C 19165-26-5, I 104-94-9
RGT G 7719-12-2 PC13
PRO J 50498-62-9
SOL 108-88-3 PhMe

RX(11) RCT J 50498-62-9
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
PRO AA 473721-15-2

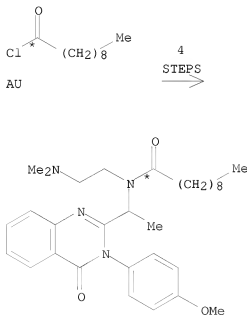
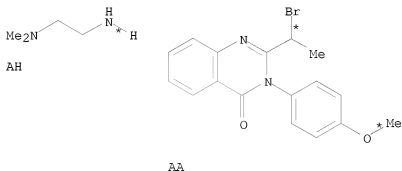
RX(19) RCT AA 473721-15-2, AH 108-00-9
PRO AK 473721-16-3
SOL 64-17-5 EtOH
CON reflux

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RX(28) RCT AK 473721-16-3, AU 112-13-0
RGT AW 121-44-8 Et3N
PRO AY 329190-30-9
SOL 123-91-1 Dioxane

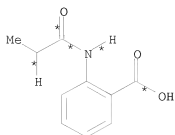
RX(35) RCT AL 329190-50-3, AY 329190-30-9, BF 2719-27-9
RGT AW 121-44-8 Et3N, AS 10294-33-4 BBr3
PRO BG 860002-99-9, BH 860003-00-5
SOL 67-56-1 MeOH, 123-91-1 Dioxane

RX(163) OF 173 COMPOSED OF REACTION SEQUENCE RX(19), RX(28), RX(35)
AND REACTION SEQUENCE RX(4), RX(12), RX(20), RX(35)
...AA + AH + AU ==> AY...
... C + K + AH + AY + BF ==> BG + BH

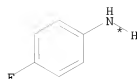


AY

START NEXT REACTION SEQUENCE



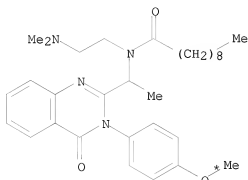
C



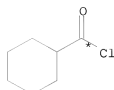
K



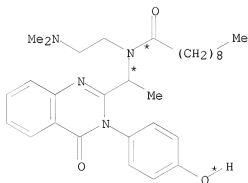
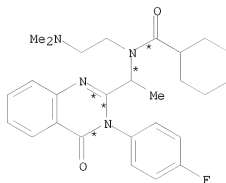
AH



AY



BF

4
STEPS
→BG
YIELD 15%BH
YIELD 55%

RX(19) RCT AA 473721-15-2, AH 108-00-9
 PRO AK 473721-16-3
 SOL 64-17-5 EtOH
 CON reflux

RX(28) RCT AK 473721-16-3, AU 112-13-0

RGT AW 121-44-8 Et3N
 PRO AY 329190-30-9
 SOL 123-91-1 Dioxane

RX(4) RCT C 19165-26-5, K 371-40-4
 RGT G 7719-12-2 PC13
 PRO L 329190-48-9
 SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AB 329190-49-0

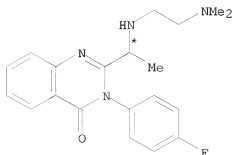
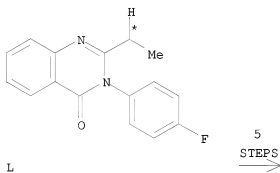
RX(20) RCT AB 329190-49-0, AH 108-00-9
 PRO AL 329190-50-3
 SOL 64-17-5 EtOH
 CON reflux

RX(35) RCT AL 329190-50-3, AY 329190-30-9, BF 2719-27-9
 RGT AW 121-44-8 Et3N, AS 10294-33-4 BBr3
 PRO BG 860002-99-9, BH 860003-00-5
 SOL 67-56-1 MeOH, 123-91-1 Dioxane

RX(166) OF 173 COMPOSED OF REACTION SEQUENCE RX(12), RX(20), RX(35)
 AND REACTION SEQUENCE RX(3), RX(11), RX(19), RX(28), RX(35)

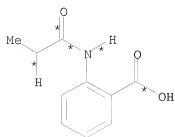
...L + AH ==> AL...

... C + I + AH + AU + AL + BF ==> BG + BH

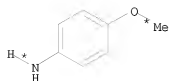


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START NEXT REACTION SEQUENCE



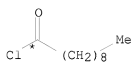
C



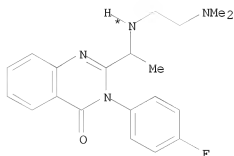
I



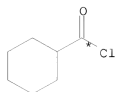
2 AH



AU

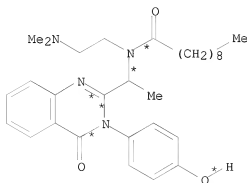


AL

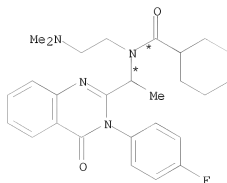


BF

5
STEPS
→



BG
YIELD 15%



BH
YIELD 55%

RX(12) RCT L 329190-48-9
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2

PRO AB 329190-49-0

RX(20) RCT AB 329190-49-0, AH 108-00-9
 PRO AL 329190-50-3
 SOL 64-17-5 EtOH
 CON reflux

RX(3) RCT C 19165-26-5, I 104-94-9
 RGT G 7719-12-2 PC13
 PRO J 50498-62-9
 SOL 108-88-3 PhMe

RX(11) RCT J 50498-62-9
 RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
 PRO AA 473721-15-2

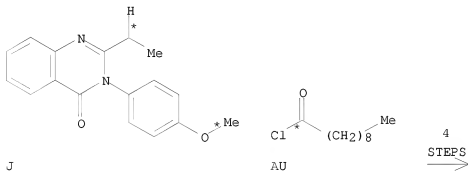
RX(19) RCT AA 473721-15-2, AH 108-00-9
 PRO AK 473721-16-3
 SOL 64-17-5 EtOH
 CON reflux

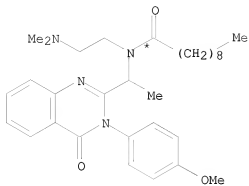
RX(28) RCT AK 473721-16-3, AU 112-13-0
 RGT AW 121-44-8 Et3N
 PRO AY 329190-30-9
 SOL 123-91-1 Dioxane

RX(35) RCT AL 329190-50-3, AY 329190-30-9, BF 2719-27-9
 RGT AW 121-44-8 Et3N, AS 10294-33-4 BBr3
 PRO BG 860002-99-9, BH 860003-00-5
 SOL 67-56-1 MeOH, 123-91-1 Dioxane

RX(168) OF 173 COMPOSED OF REACTION SEQUENCE RX(11), RX(19), RX(28), RX(35)
 AND REACTION SEQUENCE RX(4), RX(12), RX(20), RX(35)

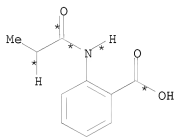
...J + AH + AU ==> AY...
 ... C + K + AH + AY + BF ==> BG + BH



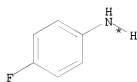


AY

START NEXT REACTION SEQUENCE



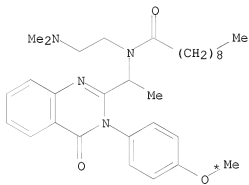
C



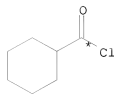
K



2 AH

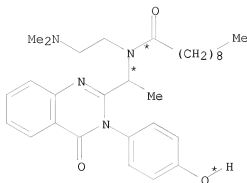


AY

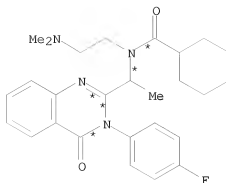


BF

4
STEPS
→



BG
YIELD 15%



BH
YIELD 55%

```

RX(11)  RCT  J 50498-62-9
        RGT  X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
        PRO  AA 473721-15-2

RX(19)  RCT  AA 473721-15-2, AH 108-00-9
        PRO  AK 473721-16-3
        SOL  64-17-5 EtOH
        CON  reflux

RX(28)  RCT  AK 473721-16-3, AU 112-13-0
        RGT  AW 121-44-8 Et3N
        PRO  AY 329190-30-9
        SOL  123-91-1 Dioxane

RX(4)   RCT  C 19165-26-5, K 371-40-4
        RGT  G 7719-12-2 PC13
        PRO  L 329190-48-9
        SOL  108-88-3 PhMe

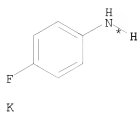
RX(12)  RCT  L 329190-48-9
        RGT  X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
        PRO  AB 329190-49-0

RX(20)  RCT  AB 329190-49-0, AH 108-00-9
        PRO  AL 329190-50-3
        SOL  64-17-5 EtOH
        CON  reflux

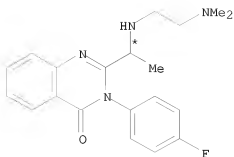
RX(35)  RCT  AL 329190-50-3, AY 329190-30-9, BF 2719-27-9
        RGT  AW 121-44-8 Et3N, AS 10294-33-4 BBr3
        PRO  BG 860002-99-9, BH 860003-00-5
        SOL  67-56-1 MeOH, 123-91-1 Dioxane

RX(170) OF 173 COMPOSED OF REACTION SEQUENCE RX(4), RX(12), RX(20), RX(35)
        AND REACTION SEQUENCE RX(3), RX(11), RX(19), RX(28), RX(35)
...  C  +  K  +  AH  ==>  AL...
...  C  +  I  +  AH  +  AU  +  AL  +  BF  ==>  BG  +  BH

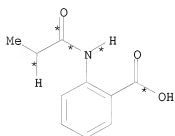
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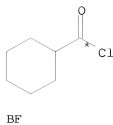
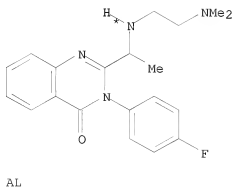
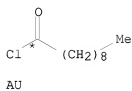
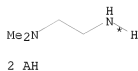
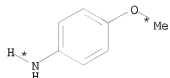
5
STEPS
→



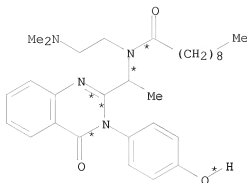
START NEXT REACTION SEQUENCE



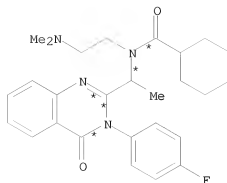
I



5
STEPS
→



BG
YIELD 15%



BH
YIELD 55%

RX(4)	RCT	C 19165-26-5, K 371-40-4
	RGT	G 7719-12-2 PC13
	PRO	L 329190-48-9
	SOL	108-88-3 PhMe
RX(12)	RCT	L 329190-48-9
	RGT	X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
	PRO	AB 329190-49-0
RX(20)	RCT	AB 329190-49-0, AH 108-00-9
	PRO	AL 329190-50-3
	SOL	64-17-5 EtOH
	CON	reflux
RX(3)	RCT	C 19165-26-5, I 104-94-9
	RGT	G 7719-12-2 PC13
	PRO	J 50498-62-9
	SOL	108-88-3 PhMe
RX(11)	RCT	J 50498-62-9
	RGT	X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
	PRO	AA 473721-15-2
RX(19)	RCT	AA 473721-15-2, AH 108-00-9
	PRO	AK 473721-16-3
	SOL	64-17-5 EtOH
	CON	reflux
RX(28)	RCT	AK 473721-16-3, AU 112-13-0
	RGT	AW 121-44-8 Et3N
	PRO	AY 329190-30-9
	SOL	123-91-1 Dioxane
RX(35)	RCT	AL 329190-50-3, AY 329190-30-9, BF 2719-27-9
	RGT	AW 121-44-8 Et3N, AS 10294-33-4 BBr3
	PRO	BG 860002-99-9, BH 860003-00-5
	SOL	67-56-1 MeOH, 123-91-1 Dioxane

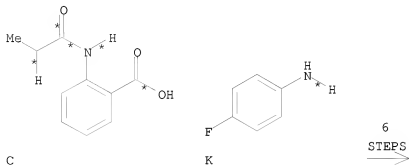
RX(171) OF 173 COMPOSED OF REACTION SEQUENCE RX(4), RX(12), RX(20), RX(35)

AND REACTION SEQUENCE RX(1), RX(3), RX(11), RX(19), RX(28),

RX(35)

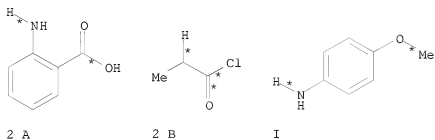
... C + K + AH ==> AL...

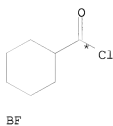
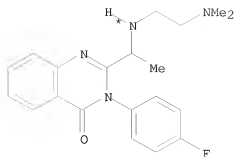
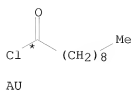
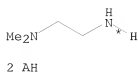
...2 A + 2 B + I + AH + AU + AL + BF ==> BG + BH



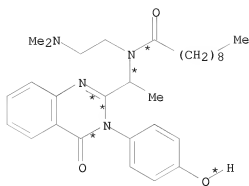
AL

START NEXT REACTION SEQUENCE

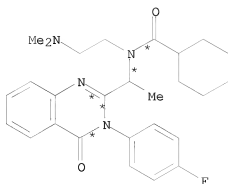




6
STEPS



YIELD 15%



YIELD 55%

RX(4) RCT C 19165-26-5, K 371-40-4
 RGT G 7719-12-2 PC13
 PRO L 329190-48-9

SOL 108-88-3 PhMe

RX(12) RCT L 329190-48-9
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
PRO AB 329190-49-0

RX(20) RCT AB 329190-49-0, AH 108-00-9
PRO AL 329190-50-3
SOL 64-17-5 EtOH
CON reflux

RX(1) RCT A 118-92-3, B 79-03-8
PRO C 19165-26-5
SOL 68-12-2 DMF

RX(3) RCT C 19165-26-5, I 104-94-9
RGT G 7719-12-2 PC13
PRO J 50498-62-9
SOL 108-88-3 PhMe

RX(11) RCT J 50498-62-9
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
PRO AA 473721-15-2

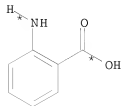
RX(19) RCT AA 473721-15-2, AH 108-00-9
PRO AK 473721-16-3
SOL 64-17-5 EtOH
CON reflux

RX(28) RCT AK 473721-16-3, AU 112-13-0
RGT AW 121-44-8 Et3N
PRO AY 329190-30-9
SOL 123-91-1 Dioxane

RX(35) RCT AL 329190-50-3, AY 329190-30-9, BF 2719-27-9
RGT AW 121-44-8 Et3N, AS 10294-33-4 BBr3
PRO BG 860002-99-9, BH 860003-00-5
SOL 67-56-1 MeOH, 123-91-1 Dioxane

RX(172) OF 173 COMPOSED OF REACTION SEQUENCE RX(1), RX(4), RX(12), RX(20),
RX(35)
AND REACTION SEQUENCE RX(3), RX(11), RX(19), RX(28), RX(35)

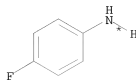
...A + B + K + AH ==> AL...
...C + I + AH + AU + AL + BF ==> BG + BH



A

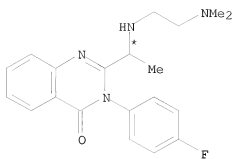


B



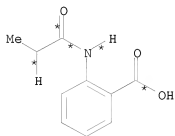
K

5
STEPS
→

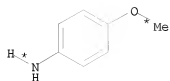


AL

START NEXT REACTION SEQUENCE



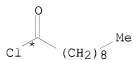
C



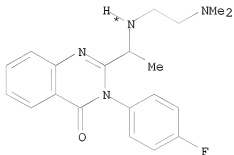
I



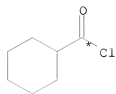
2 AH



AU

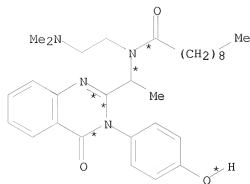


AL

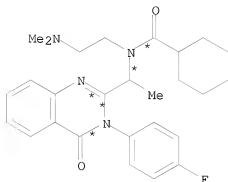


BF

5
STEPS
→



BG
YIELD 15%



BH
YIELD 55%

RX(1)	RCT	A 118-92-3, B 79-03-8	
	PRO	C 19165-26-5	
	SOL	68-12-2 DMF	
RX(4)	RCT	C 19165-26-5, K 371-40-4	
	RGT	G 7719-12-2 PC13	
	PRO	L 329190-48-9	
	SOL	108-88-3 PhMe	
RX(12)	RCT	L 329190-48-9	
	RGT	X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2	
	PRO	AB 329190-49-0	
RX(20)	RCT	AB 329190-49-0, AH 108-00-9	
	PRO	AL 329190-50-3	
	SOL	64-17-5 EtOH	
	CON	reflux	
RX(3)	RCT	C 19165-26-5, I 104-94-9	
	RGT	G 7719-12-2 PC13	

PRO J 50498-62-9
SOL 108-88-3 PhMe

RX(11) RCT J 50498-62-9
RGT X 127-09-3 AcONa, Y 64-19-7 AcOH, Z 7726-95-6 Br2
PRO AA 473721-15-2

RX(19) RCT AA 473721-15-2, AH 108-00-9
PRO AK 473721-16-3
SOL 64-17-5 EtOH
CON reflux

RX(28) RCT AK 473721-16-3, AU 112-13-0
RGT AW 121-44-8 Et3N
PRO AY 329190-30-9
SOL 123-91-1 Dioxane

RX(35) RCT AL 329190-50-3, AY 329190-30-9, BF 2719-27-9
RGT AW 121-44-8 Et3N, AS 10294-33-4 BBr3
PRO BG 860002-99-9, BH 860003-00-5
SOL 67-56-1 MeOH, 123-91-1 Dioxane

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 50 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 143:26556 CASREACT

TITLE: Synthetic studies on 3-arylquinazolin-4-ones:
intramolecular nucleophilic aromatic substitution
reaction of 2-carboxamido-3-arylquinazolin-4-ones and
its application to the synthesis of secondary aryl
amines

AUTHOR(S): Fuwa, Haruhiko; Kobayashi, Toshitake; Tokitoh,

CORPORATE SOURCE: Takashi; Torii, Yukiko; Natsugari, Hideaki
Graduate School of Pharmaceutical Sciences, University
of Tokyo, Bunkyo-ku, Tokyo, 113-0033, Japan

SOURCE: Tetrahedron (2005), 61(17), 4297-4312

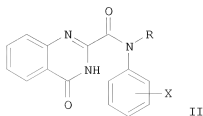
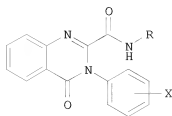
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

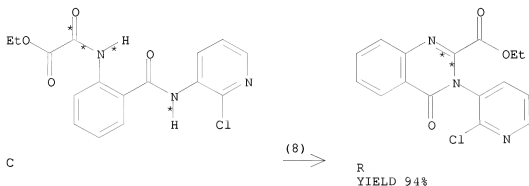
LANGUAGE: English

GI



AB 2-Carboxamido-3-arylquinazolin-4-ones were prepared via acylation of aromatic amines, cyclodehydration, transesterification, and amidation. A novel intramol. nucleophilic aromatic substitution (SNAr) reaction of 2-carboxamido-3-arylquinazolin-4-ones, a potentially useful scaffold in the field of medicinal chemical, is described. E.g., treatment of 2-carboxamido-3-arylquinazolin-4-ones I (X = 4-CF₃, o-CO₂Me, 4-CN, etc.; R = CH₂Ph, Ph, Bu) with NaH in DMF gave migrated products II. The synthetic utility of the SNAr reaction as a tool for the synthesis of secondary aryl amines, including diaryl amines, is also demonstrated. Thus, reaction of the 2-ethoxycarbonyl-3-arylquinazolin-4-ones and primary amines in the presence of a base induced a cascade process comprised of amide formation, intramol. SNAr reaction, and cleavage of the resultant tertiary amide to yield (in one-pot) secondary aryl amines.

RX(8) OF 229 ...C ==> R...



RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)₂, T 7553-56-2 I₂, U 603-35-0 PPh₃

SOL 75-09-2 CH₂Cl₂

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

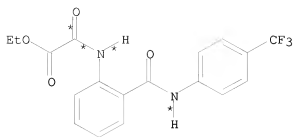
RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

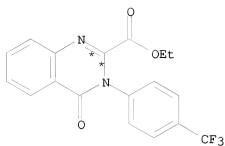
RX(9) OF 229 ...G ==> X...

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G

(9) \longrightarrow



X

YIELD 82%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

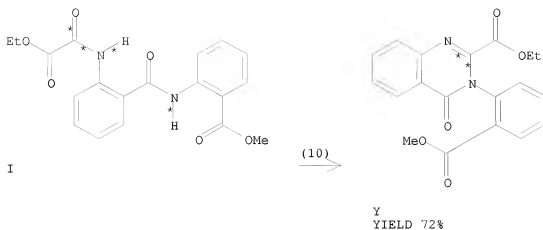
RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO X 361180-29-2

RX(10) OF 229 ...I ==> Y...

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RX(10) RCT I 852534-80-6

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

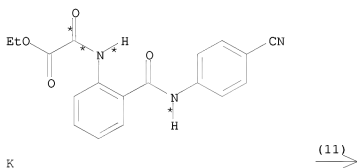
STAGE(2)

RGT V 123-75-1 Pyrrolidine

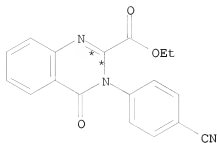
SOL 109-99-9 THF

PRO Y 852534-83-9

RX(11) OF 229 ...K ==> Z...



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Z
YIELD 60%

RX(11) RCT K 852534-81-7

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

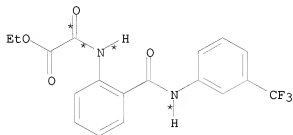
STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO Z 830325-00-3

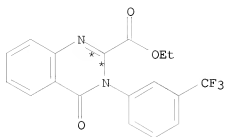
RX(12) OF 229 ...M ==> AA...



M

(12)

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AA

YIELD 77%

RX(12) RCT M 852534-82-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

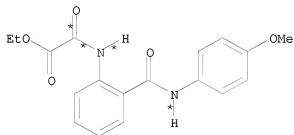
STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO AA 310423-02-0

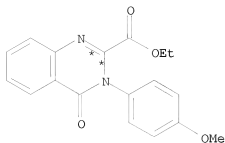
RX(13) OF 229 ...O ==> AB...



O

(13)

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AB
YIELD 46%

RX(13) RCT O 30838-15-4

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

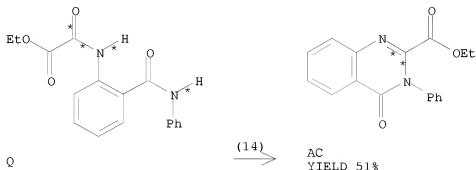
STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO AB 30838-19-8

RX(14) OF 229 ...Q ==> AC...



RX(14) RCT Q 30838-11-0

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

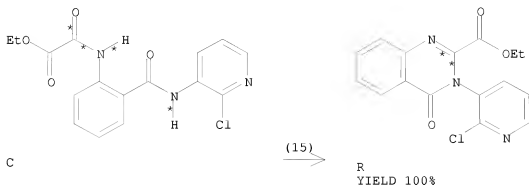
RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

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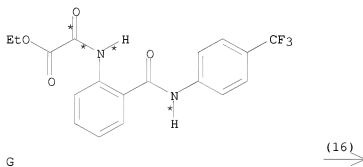
PRO AC 30838-16-5

RX(15) OF 229 C ==> R

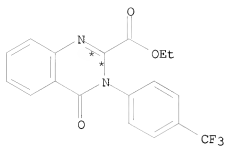


RX(15) RCT C 830324-66-8
RGT AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl
PRO R 830324-68-0
SOL 107-06-2 ClCH2CH2Cl
CON 1.5 hours, reflux

RX(16) OF 229 G ==> X



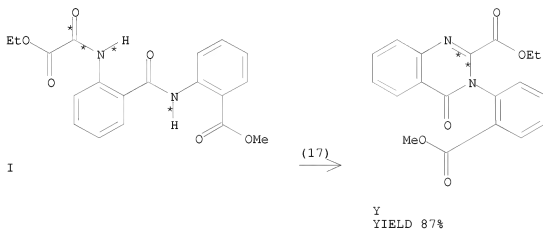
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X
YIELD 94%

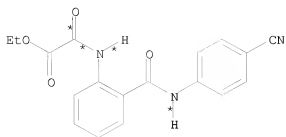
RX(16) RCT G 852534-79-3
RGT AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl
PRO X 361180-29-2
SOL 107-06-2 ClCH2CH2Cl
CON 1.5 hours, reflux

RX(17) OF 229 I ==> Y



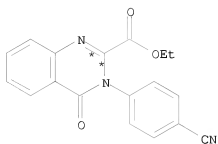
RX(17) RCT I 852534-80-6
RGT AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl
PRO Y 852534-83-9
SOL 107-06-2 ClCH2CH2Cl
CON 1.5 hours, reflux

RX(18) OF 229 K ==> Z



K

(18) \longrightarrow

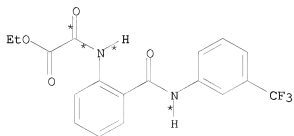


Z

YIELD 89%

RX(18) RCT K 852534-81-7
 RGT AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl
 PRO Z 830325-00-3
 SOL 107-06-2 ClCH2CH2Cl
 CON 1.5 hours, reflux

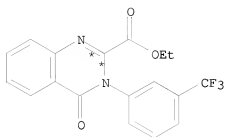
RX(19) OF 229 M \implies AA



M

(19) \longrightarrow

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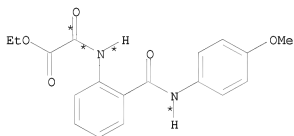


AA

YIELD 98%

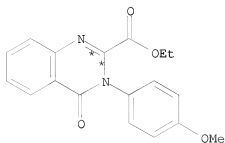
RX(19) RCT M 852534-82-8
RGT AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl
PRO AA 310423-02-0
SOL 107-06-2 ClCH2CH2Cl
CON 1.5 hours, reflux

RX(20) OF 229 O ==> AB



O

(20)



AB

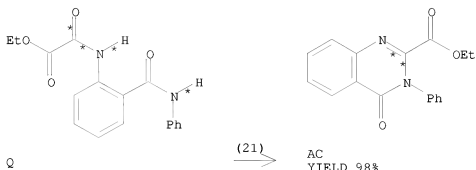
YIELD 84%

RX(20) RCT O 30838-15-4

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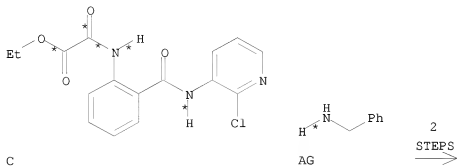
RGT AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl
 PRO AB 30838-19-8
 SOL 107-06-2 ClCH2CH2Cl
 CON 1.5 hours, reflux

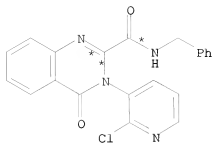
RX(21) OF 229 Q ==> AC



RX(21) RCT Q 30838-11-0
 RGT AD 121-44-8 Et3N, AE 75-77-4 Me3SiCl
 PRO AC 30838-16-5
 SOL 107-06-2 ClCH2CH2Cl
 CON 1.5 hours, reflux

RX(80) OF 229 COMPOSED OF RX(8), RX(22)
 RX(80) C + AG ==> AH





AH
YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO R 830324-68-0

RX(22) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 1 hour, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0
CON 7 hours, room temperature

STAGE(3)

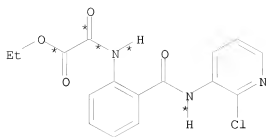
RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AH 830324-76-0

RX(81) OF 229 COMPOSED OF RX(8), RX(38)

RX(81) C + BM ==> AR

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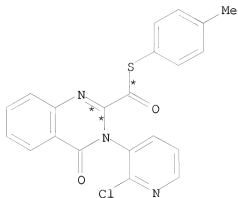


C



BM

2
STEPS
→



AR
YIELD 87%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

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STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

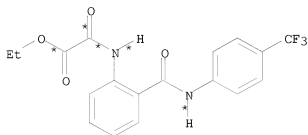
SOL 7732-18-5 Water

CON 0 deg C

PRO AR 830324-69-1

RX(88) OF 229 COMPOSED OF RX(9), RX(23)

RX(88) G + AG ==> AM

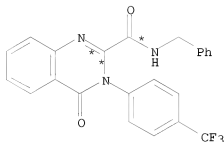


G



AG

2
STEPS
→



AM

YIELD 76%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)₂, T 7553-56-2 I₂, U 603-35-0 PPh₃

SOL 75-09-2 CH₂Cl₂

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

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PRO X 361180-29-2

RX(23) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 1 hour, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2

CON 7 hours, room temperature

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

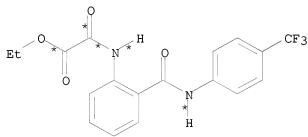
SOL 7732-18-5 Water

CON 0 deg C

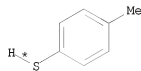
PRO AM 830324-84-0

RX(89) OF 229 COMPOSED OF RX(9), RX(39)

RX(89) G + BM ==> AZ

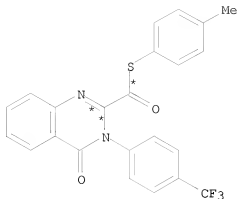


G



BM

2
STEPS
→



AZ
YIELD 60%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO X 361180-29-2

RX(39) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

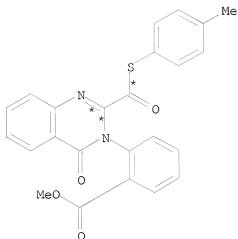
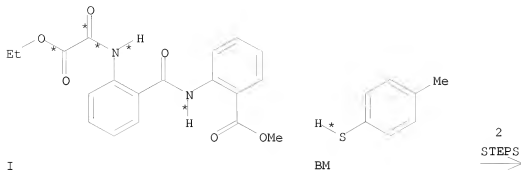
RCT X 361180-29-2
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AZ 852534-84-0

RX(92) OF 229 COMPOSED OF RX(10), RX(40)
RX(92) I + BM ==> AV



YIELD 91%

RX(10) RCT I 852534-80-6

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
 SOL 109-99-9 THF

PRO Y 852534-83-9

RX(40) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
 SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
 CON SUBSTAGE(1) 0 deg C

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SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Y 852534-83-9

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

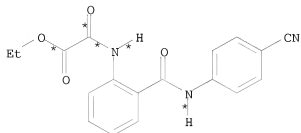
SOL 7732-18-5 Water

CON 0 deg C

PRO AV 852534-85-1

RX(93) OF 229 COMPOSED OF RX(11), RX(24)

RX(93) K + AG ==> AN

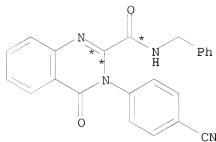


K



AG

2
STEPS
→



AN

YIELD 53%

RX(11) RCT K 852534-81-7

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

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RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO Z 830325-00-3

RX(24) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe₃
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 1 hour, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Z 830325-00-3
CON 7 hours, room temperature

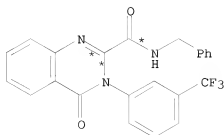
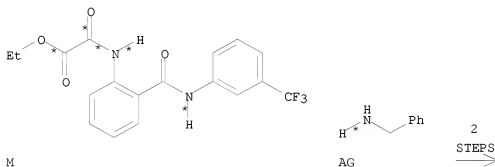
STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AN 830324-86-2

RX(96) OF 229 COMPOSED OF RX(12), RX(25)

RX(96) M + AG ==> AO



AO
YIELD 93%

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RX(12) RCT M 852534-82-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO AA 310423-02-0

RX(25) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 1 hour, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT AA 310423-02-0
CON 7 hours, room temperature

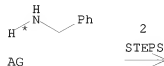
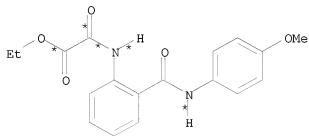
STAGE(3)

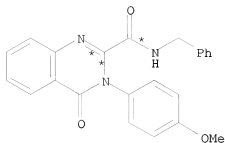
RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AO 852534-86-2

RX(97) OF 229 COMPOSED OF RX(13), RX(26)

RX(97) O + AG ==> AP





AP
YIELD 96%

RX(13) RCT O 30838-15-4

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO AB 30838-19-8

RX(26) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 1 hour, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT AB 30838-19-8
CON 7 hours, room temperature

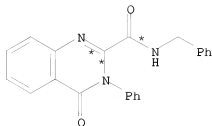
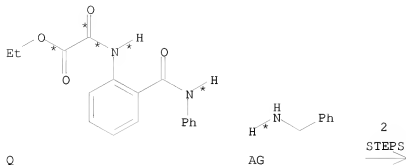
STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AP 852534-87-3

RX(98) OF 229 COMPOSED OF RX(14), RX(27)

RX(98) Q + AG ==> AQ



YIELD 78%

RX(14) RCT Q 30838-11-0

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO AC 30838-16-5

RX(27) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 1 hour, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT AC 30838-16-5

CON 7 hours, room temperature

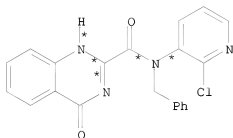
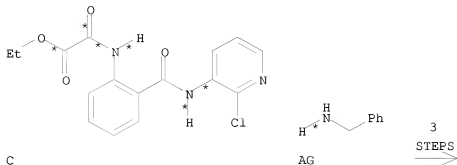
STAGE(3)

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RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AQ 852534-88-4

RX(151) OF 229 COMPOSED OF RX(8), RX(22), RX(43)
RX(151) C + AG ==> BU



BU
YIELD 85%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO R 830324-68-0

RX(22) RCT AG 100-46-9

STAGE(1)

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RGT AI 75-24-1 AlMe₃
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 1 hour, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)
RCT R 830324-68-0
CON 7 hours, room temperature

STAGE(3)
RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AH 830324-76-0

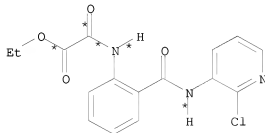
RX(43) RCT AH 830324-76-0

STAGE(1)
RGT BR 7646-69-7 NaH
SOL 108-88-3 PhMe
CON overnight, 80 deg C

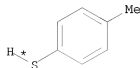
STAGE(2)
RGT BS 12125-02-9 NH₄Cl
SOL 7732-18-5 Water

PRO BU 830324-81-7
NTE optimization study

RX(153) OF 229 COMPOSED OF RX(8), RX(38), RX(28)
RX(153) C + BM + AG ==> AH



C



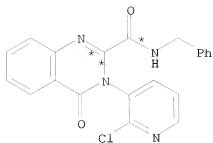
BM



AG

3
STEPS
→

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AH
YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AR 830324-69-1

RX(28) RCT AG 100-46-9, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

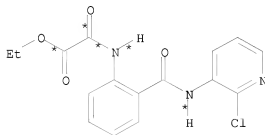
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

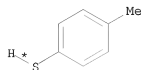
PRO AH 830324-76-0

RX(154) OF 229 COMPOSED OF RX(8), RX(38), RX(30)

RX(154) C + BM + AX ==> AY



C

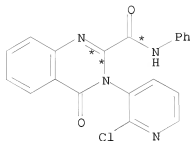


BM



AX

3
STEPS
=>



AY

YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

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PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AR 830324-69-1

RX(30) RCT AX 62-53-3, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

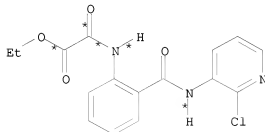
STAGE(2)

RGT AT 1336-21-6 NH4OH
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 10 minutes, room temperature

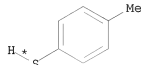
PRO AY 830324-73-7

RX(155) OF 229 COMPOSED OF RX(8), RX(38), RX(33)

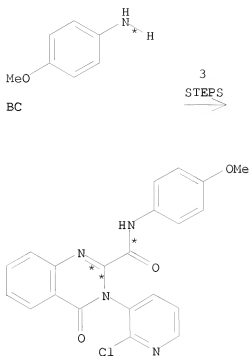
RX(155) C + BM + BC ==> BD



C



BM



BD
YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

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STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AR 830324-69-1

RX(33) RCT BC 104-94-9, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

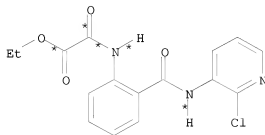
STAGE(2)

RGT AT 1336-21-6 NH4OH
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 10 minutes, room temperature

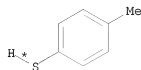
PRO BD 830324-74-8

RX(156) OF 229 COMPOSED OF RX(8), RX(38), RX(34)

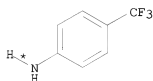
RX(156) C + BM + BE ==> BF



C

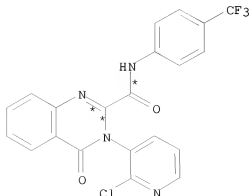


BM



BE

3
STEPS
→



BF
YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AR 830324-69-1

RX(34) RCT BE 455-14-1, AR 830324-69-1

STAGE(1)

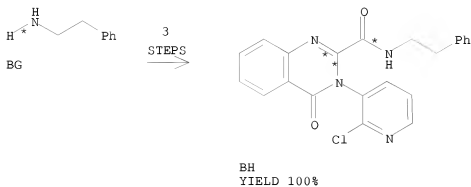
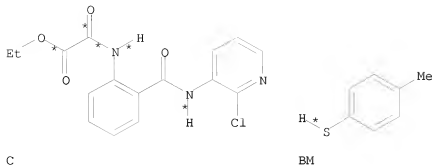
RGT AS 2966-50-9 F3CCO2 Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

RGT AT 1336-21-6 NH4OH
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 10 minutes, room temperature

PRO BF 830324-75-9

RX(157) OF 229 COMPOSED OF RX(8), RX(38), RX(35)
RX(157) C + BM + BG ==> BH



RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
 SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
 SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 30 minutes, room temperature
 SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0
 CON SUBSTAGE(1) 80 minutes, room temperature
 SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
 SOL 7732-18-5 Water
 CON 0 deg C

PRO AR 830324-69-1

RX(35) RCT BG 64-04-0, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag
 SOL 109-99-9 THF, 108-88-3 PhMe
 CON SUBSTAGE(1) 1.5 hours, 60 deg C
 SUBSTAGE(2) 60 deg C -> room temperature

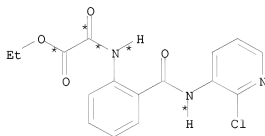
STAGE(2)

RGT AT 1336-21-6 NH4OH
 SOL 7732-18-5 Water, 75-09-2 CH2Cl2
 CON 10 minutes, room temperature

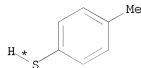
PRO BH 830324-77-1

RX(158) OF 229 COMPOSED OF RX(8), RX(38), RX(37)

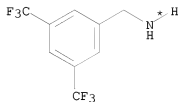
RX(158) C + BM + BK ==> BL



C

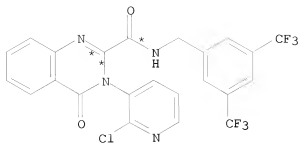


BM



BK

3
 STEPS
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BL
YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)₂, T 7553-56-2 I₂, U 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe₃
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AR 830324-69-1

RX(37) RCT AR 830324-69-1, BK 85068-29-7

STAGE(1)

RGT AS 2966-50-9 F₃CCO₂ Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

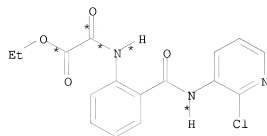
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

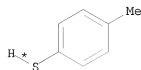
PRO BL 830324-70-4

RX(159) OF 229 COMPOSED OF RX(8), RX(38), RX(41)

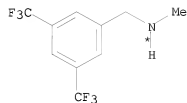
RX(159) C + BM + BN ==> BO



C

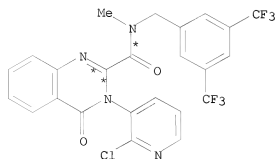


BM



BN

3
STEPS
→



BO

YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)
RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)
RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)
RCT R 830324-68-0
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)
RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AR 830324-69-1

RX(41) RCT AR 830324-69-1, BN 159820-24-3

STAGE(1)
RGT AS 2966-50-9 F3CCO2 Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

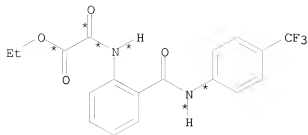
STAGE(2)
RGT AT 1336-21-6 NH4OH
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 10 minutes, room temperature

PRO BO 830324-71-5

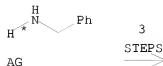
RX(169) OF 229 COMPOSED OF RX(9), RX(23), RX(48)

RX(169) G + AG ==> BZ

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G



BZ
YIELD 95%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO X 361180-29-2

RX(23) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 1 hour, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2
CON 7 hours, room temperature

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STAGE (3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AM 830324-84-0

RX (48) RCT AM 830324-84-0

STAGE (1)

RGT BR 7646-69-7 NaH

SOL 68-12-2 DMF

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CON SUBSTAGE(1) 0 deg C -> room temperature
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SUBSTAGE (2) 1 hour, room temperature

STAGE (2)

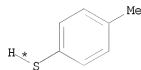
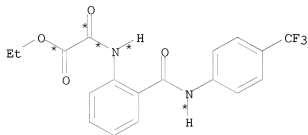
RGT BS 12125-02-9 NH4Cl

SOL 7732-18-5 Water

CON 0 deg C

PRO BZ 830324-91-9

RX(170) OF 229 COMPOSED OF RX(9), RX(39), RX(31)

$$\text{RX(170)} \quad \text{G} \quad + \quad \text{BM} \quad + \quad \text{AX} \quad \Longrightarrow \quad \text{BA}$$


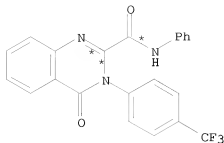
G

BM



AX

3
STEPS
→



BA
YIELD 81%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO X 361180-29-2

RX(39) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AZ 852534-84-0

RX(31) RCT AX 62-53-3, AZ 852534-84-0

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

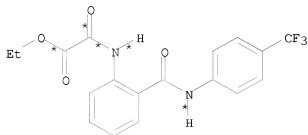
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

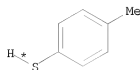
PRO BA 830324-83-9

RX(171) OF 229 COMPOSED OF RX(9), RX(39), RX(36)

RX(171) G + BM + BI ==> BJ



G

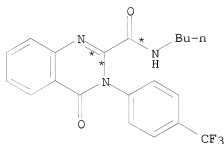


BM



BI

3
STEPS
→



BJ

YIELD 96%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

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SOL 109-99-9 THF

PRO X 361180-29-2

RX(39) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AZ 852534-84-0

RX(36) RCT BI 109-73-9, AZ 852534-84-0

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

RGT AT 1336-21-6 NH4OH

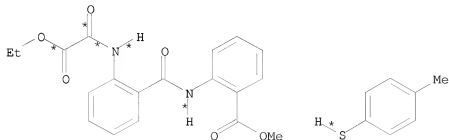
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO BJ 830324-85-1

RX(175) OF 229 COMPOSED OF RX(10), RX(40), RX(29)

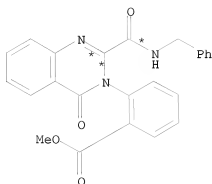
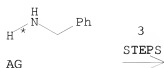
RX(175) I + BM + AG ==> AW



I

BM

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AG
YIELD 100%

RX(10) RCT I 852534-80-6

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO Y 852534-83-9

RX(40) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Y 852534-83-9
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

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PRO AV 852534-85-1

RX(29) RCT AG 100-46-9, AV 852534-85-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

RGT AT 1336-21-6 NH4OH

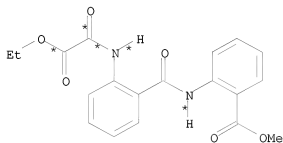
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

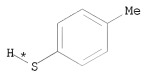
PRO AW 830324-89-5

RX(176) OF 229 COMPOSED OF RX(10), RX(40), RX(32)

RX(176) I + BM + AX ==> BB



I

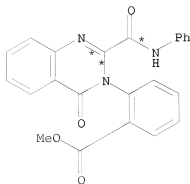


BM



AX

3
STEPS
→



BB
YIELD 87%

RX(10) RCT I 852534-80-6

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO Y 852534-83-9

RX(40) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Y 852534-83-9
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AV 852534-85-1

RX(32) RCT AX 62-53-3, AV 852534-85-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

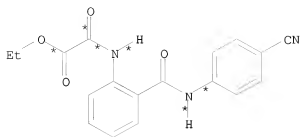
RGT AT 1336-21-6 NH4OH
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 10 minutes, room temperature

PRO BB 830324-87-3

RX(179) OF 229 COMPOSED OF RX(11), RX(24), RX(53)

RX(179) K + AG ==> CE

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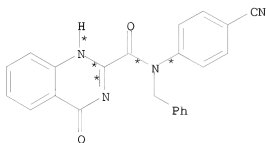


K



AG

3
STEPS
→



CE

YIELD 95%

RX(11) RCT K 852534-81-7

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO Z 830325-00-3

RX(24) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 1 hour, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Z 830325-00-3

CON 7 hours, room temperature

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STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AN 830324-86-2

RX(53) RCT AN 830324-86-2

STAGE(1)

RGT BR 7646-69-7 NaH
SOL 68-12-2 DMF
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

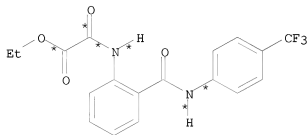
STAGE(2)

RGT BS 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON 0 deg C

PRO CE 830324-93-1

RX(182) OF 229 COMPOSED OF RX(9), RX(23), RX(48), RX(57)

RX(182) G + AG + BP ==> CK



G

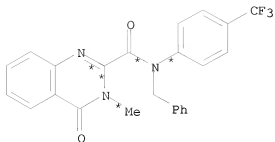


AG



BP

4
STEPS
→



CK
YIELD 92%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO X 361180-29-2

RX(23) RCT AG 100-46-9

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 1 hour, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2
CON 7 hours, room temperature

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AM 830324-84-0

RX(48) RCT AM 830324-84-0

STAGE(1)

RGT BR 7646-69-7 NaH
SOL 68-12-2 DMF
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

10/ 562,112

RGT BS 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON 0 deg C

PRO BZ 830324-91-9

RX(57) RCT BZ 830324-91-9, BP 74-88-4

STAGE(1)

RGT BR 7646-69-7 NaH
SOL 68-12-2 DMF
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

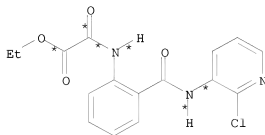
STAGE(2)

RGT BS 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON 0 deg C

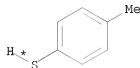
PRO CK 830324-99-7

RX(194) OF 229 COMPOSED OF RX(8), RX(38), RX(28), RX(43)

RX(194) C + BM + AG ==> BU



C



BM

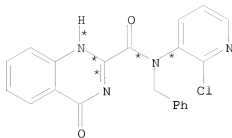


AG

4

STEPS





BU
YIELD 85%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AR 830324-69-1

RX(28) RCT AG 100-46-9, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO AH 830324-76-0

RX(43) RCT AH 830324-76-0

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 108-88-3 PhMe

CON overnight, 80 deg C

STAGE(2)

RGT BS 12125-02-9 NH4Cl

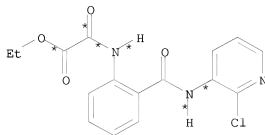
SOL 7732-18-5 Water

PRO BU 830324-81-7

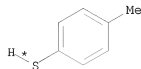
NTE optimization study

RX(196) OF 229 COMPOSED OF RX(8), RX(38), RX(30), RX(44)

RX(196) C + BM + AX ==> BV



C



BM

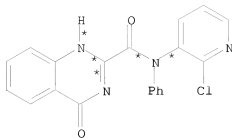


AX

4

STEPS





BV

YIELD 88%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AR 830324-69-1

RX(30) RCT AX 62-53-3, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

SOL 109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) 1.5 hours, 60 deg C

SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO AY 830324-73-7

RX(44) RCT AY 830324-73-7

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RGT BS 12125-02-9 NH4Cl

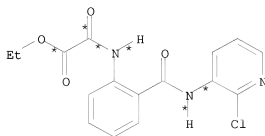
SOL 7732-18-5 Water

CON 0 deg C

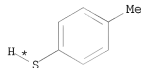
PRO BV 830324-78-2

RX(198) OF 229 COMPOSED OF RX(8), RX(38), RX(33), RX(45)

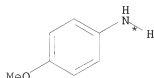
RX(198) C + BM + BC ==> BW



C

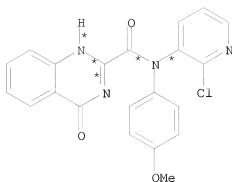


BM



BC

4
STEPS
→



BW

YIELD 87%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine

SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3

SOL 75-09-2 CH2Cl2, 110-54-3 Hexane

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) 30 minutes, room temperature

SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0

CON SUBSTAGE(1) 80 minutes, room temperature

SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt

SOL 7732-18-5 Water

CON 0 deg C

PRO AR 830324-69-1

RX(33) RCT BC 104-94-9, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

SOL 109-99-9 THF, 108-88-3 PhMe

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CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

RGT AT 1336-21-6 NH4OH
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 10 minutes, room temperature

PRO BD 830324-74-8

RX(45) RCT BD 830324-74-8

STAGE(1)

RGT BR 7646-69-7 NaH
SOL 68-12-2 DMF
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

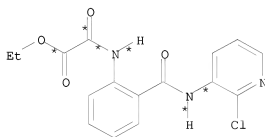
STAGE(2)

RGT BS 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON 0 deg C

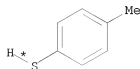
PRO BW 830324-79-3

RX(200) OF 229 COMPOSED OF RX(8), RX(38), RX(34), RX(46)

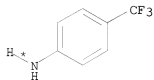
RX(200) C + BM + BE ==> BX



C

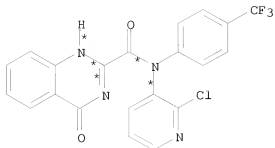


BM



BE

4
STEPS
→



BX
YIELD 100%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AR 830324-69-1

RX(34) RCT BE 455-14-1, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO BF 830324-75-9

RX(46) RCT BF 830324-75-9

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RGT BS 12125-02-9 NH4Cl

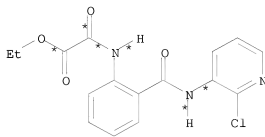
SOL 7732-18-5 Water

CON 0 deg C

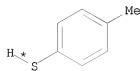
PRO BX 830324-80-6

RX(202) OF 229 COMPOSED OF RX(8), RX(38), RX(35), RX(47)

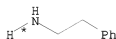
RX(202) C + BM + BG ==> BY



C

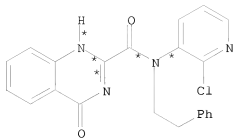


BM



BG

4
STEPS
→



BY
YIELD 63%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AR 830324-69-1

RX(35) RCT BG 64-04-0, AR 830324-69-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO BH 830324-77-1

RX(47) RCT BH 830324-77-1

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RGT BS 12125-02-9 NH4Cl

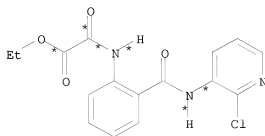
SOL 7732-18-5 Water

CON 0 deg C

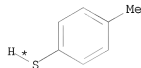
PRO BY 830324-82-8

RX(204) OF 229 COMPOSED OF RX(8), RX(38), RX(37), RX(42)

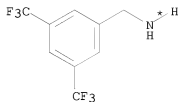
RX(204) C + BM + BK + BP ==> BQ



C



BM

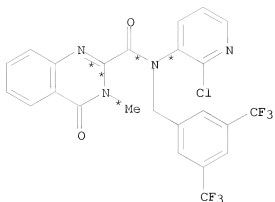


BK



BP

4
STEPS
=>



BQ
YIELD 81%

RX(8) RCT C 830324-66-8

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO R 830324-68-0

RX(38) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT R 830324-68-0
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AR 830324-69-1

RX(37) RCT AR 830324-69-1, BK 85068-29-7

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag

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SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

RGT AT 1336-21-6 NH4OH
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON 10 minutes, room temperature

PRO BL 830324-70-4

RX(42) RCT BL 830324-70-4

STAGE(1)

RGT BR 7646-69-7 NaH
SOL 68-12-2 DMF
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RCT BP 74-88-4
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 1 hour, room temperature

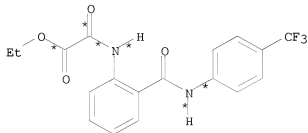
STAGE(3)

RGT BS 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON 0 deg C

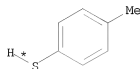
PRO BQ 830324-72-6

RX(207) OF 229 COMPOSED OF RX(9), RX(39), RX(31), RX(49)

RX(207) G + BM + AX ==> CA



G

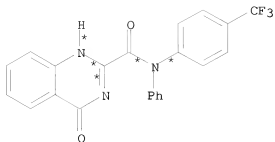


BM



AX

4
STEPS
➡



CA
YIELD 85%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)₂, T 7553-56-2 I₂, U 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO X 361180-29-2

RX(39) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe₃
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AZ 852534-84-0

RX(31) RCT AX 62-53-3, AZ 852534-84-0

STAGE(1)

RGT AS 2966-50-9 F₃CCO₂ Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO BA 830324-83-9

RX(49) RCT BA 830324-83-9

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RGT BS 12125-02-9 NH4Cl

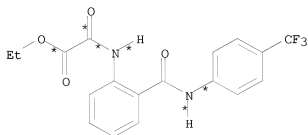
SOL 7732-18-5 Water

CON 0 deg C

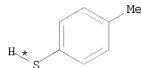
PRO CA 830324-90-8

RX(208) OF 229 COMPOSED OF RX(9), RX(39), RX(36), RX(50)

RX(208) G + BM + BI ==> CB



G

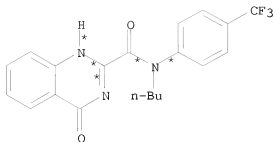


BM



BI

4
STEPS
→



CB
YIELD 100%

RX(9) RCT G 852534-79-3

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)₂, T 7553-56-2 I₂, U 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO X 361180-29-2

RX(39) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe₃
SOL 75-09-2 CH₂Cl₂, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT X 361180-29-2
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AZ 852534-84-0

RX(36) RCT BI 109-73-9, AZ 852534-84-0

STAGE(1)

RGT AS 2966-50-9 F₃CCO₂ Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO BJ 830324-85-1

RX(50) RCT BJ 830324-85-1

STAGE(1)

RGT BR 7646-69-7 NaH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RGT BS 12125-02-9 NH4Cl

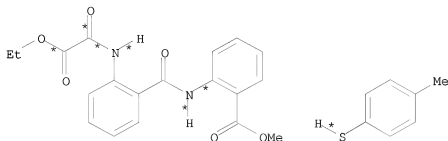
SOL 7732-18-5 Water

CON 0 deg C

PRO CB 830324-92-0

RX(211) OF 229 COMPOSED OF RX(10), RX(40), RX(29), RX(51)

RX(211) I + BM + AG ==> CC



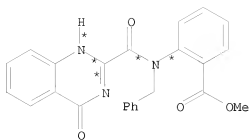
I

BM



AG

4
STEPS
→



CC
YIELD 100%

RX(10) RCT I 852534-80-6

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO Y 852534-83-9

RX(40) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Y 852534-83-9
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AV 852534-85-1

RX(29) RCT AG 100-46-9, AV 852534-85-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

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STAGE(2)

RGT AT 1336-21-6 NH4OH

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

CON 10 minutes, room temperature

PRO AW 830324-89-5

RX(51) RCT AW 830324-89-5

STAGE(1)

RGT BR 7646-69-7 NaNH

SOL 68-12-2 DMF

CON SUBSTAGE(1) 0 deg C -> room temperature

SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RGT BS 12125-02-9 NH4Cl

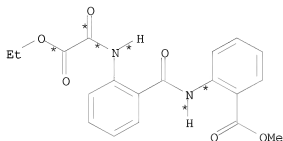
SOL 7732-18-5 Water

CON 0 deg C

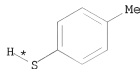
PRO CC 830324-96-4

RX(212) OF 229 COMPOSED OF RX(10), RX(40), RX(32), RX(52)

RX(212) I + BM + AX ==> CD



I



BM

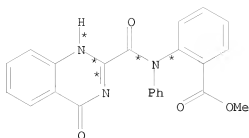


AX

4

STEPS





CD
YIELD 72%

RX(10) RCT I 852534-80-6

STAGE(1)

RGT S 7087-68-5 EtN(Pr-i)2, T 7553-56-2 I2, U 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 50 minutes, room temperature

STAGE(2)

RGT V 123-75-1 Pyrrolidine
SOL 109-99-9 THF

PRO Y 852534-83-9

RX(40) RCT BM 106-45-6

STAGE(1)

RGT AI 75-24-1 AlMe3
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 30 minutes, room temperature
SUBSTAGE(3) room temperature -> 0 deg C

STAGE(2)

RCT Y 852534-83-9
CON SUBSTAGE(1) 80 minutes, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(3)

RGT AJ 304-59-6 Rochelle salt
SOL 7732-18-5 Water
CON 0 deg C

PRO AV 852534-85-1

RX(32) RCT AX 62-53-3, AV 852534-85-1

STAGE(1)

RGT AS 2966-50-9 F3CCO2 Ag
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) 1.5 hours, 60 deg C
SUBSTAGE(2) 60 deg C -> room temperature

STAGE(2)

RGT AT 1336-21-6 NH4OH
 SOL 7732-18-5 Water, 75-09-2 CH2Cl2
 CON 10 minutes, room temperature

PRO BB 830324-87-3

RX(52) RCT BB 830324-87-3

STAGE(1)

RGT BR 7646-69-7 NaH
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 0 deg C -> room temperature
 SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RGT BS 12125-02-9 NH4Cl
 SOL 7732-18-5 Water
 CON 0 deg C

PRO CD 830324-94-2

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 51 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 143:336 CASREACT

TITLE: Identification of chemokine receptor CCR4 antagonist

AUTHOR(S): Purandare, Ashok V.; Gao, Aiming; Wan, Honghe;
 Somerville, John; Burke, Christine; Seachord, Carrie;
 Vaccaro, Wayne; Wityak, John; Poss, Michael A.

CORPORATE SOURCE: Bristol-Myers Squibb Pharmaceutical Research
 Institute, Princeton, NJ, 08543, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005),
 15(10), 2669-2672

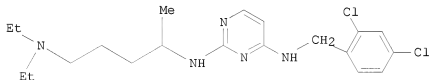
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

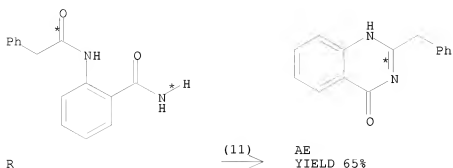


I

AB The present study reports the identification and hits to leads
 optimization of chemokine receptor CCR4 antagonists. Compound I is a high
 affinity, noncytotoxic antagonist of CCR4 that blocks the functional
 activity mediated by the receptor.

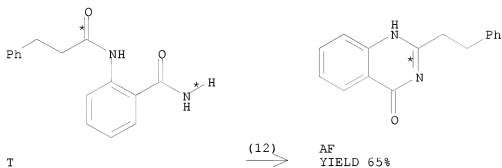
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RX(11) OF 68 ...R ==> AE...



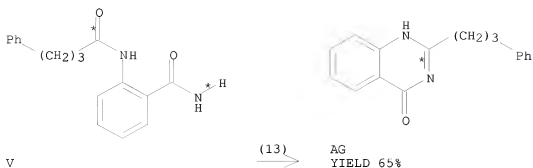
RX(11) RCT R 52910-86-8
RGT AB 141-52-6 NaOEt, AC 7722-84-1 H2O2
PRO AE 4765-56-4
CON room temperature

RX(12) OF 68 ...T ==> AF...



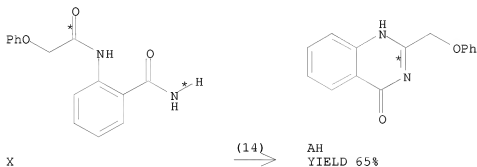
RX(12) RCT T 313382-30-8
RGT AB 141-52-6 NaOEt, AC 7722-84-1 H2O2
PRO AF 4765-57-5
CON room temperature

RX(13) OF 68 ...V ==> AG...



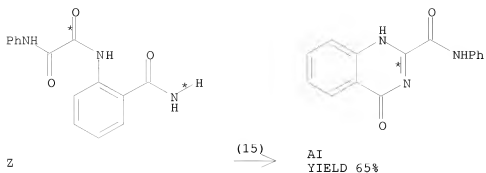
RX(13) RCT V 430453-70-6
RGT AB 141-52-6 NaOEt, AC 7722-84-1 H2O2
PRO AG 852460-38-9
CON room temperature

RX(14) OF 68 ...X ==> AH...



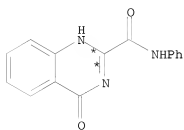
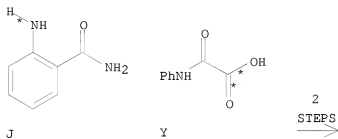
RX(14) RCT X 52910-87-9
RGT AB 141-52-6 NaOEt, AC 7722-84-1 H2O2
PRO AH 100880-66-8
CON room temperature

RX(15) OF 68 ...Z ==> AI...



RX(15) RCT Z 852460-37-8
RGT AB 141-52-6 NaOEt, AC 7722-84-1 H2O2
PRO AI 118372-87-5
CON room temperature

RX(52) OF 68 COMPOSED OF RX(8), RX(15)
RX(52) J + Y ==> AI



AI
YIELD 65%

RX(8) RCT J 88-68-6, Y 500-72-1
RGT M 25952-53-8 EDAP
PRO Z 852460-37-8
SOL 75-09-2 CH2Cl2
CON room temperature

RX(15) RCT Z 852460-37-8

RGT AB 141-52-6 NaOEt, AC 7722-84-1 H2O2
 PRO AI 118372-87-5
 CON room temperature

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 52 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:447174 CASREACT

TITLE: Synthesis and antimicrobial activity of
 2-[1-(4-chlorophenyl)-2-methylpropyl]-3-arylquinazolin-
 4(3H)-ones

AUTHOR(S): Radadia, V. R.; Purohit, D. M.; Patolia, V. N.

CORPORATE SOURCE: India

SOURCE: Indian Journal of Heterocyclic Chemistry (2004),

14(2), 153-154

CODEN: IJCHEI; ISSN: 0971-1627

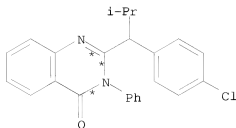
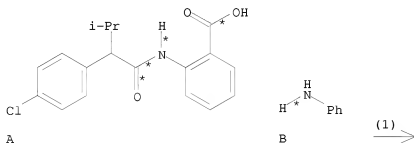
PUBLISHER: Prof. R. S. Varma

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The title compds. were prepared by the chemoselective cyclocondensation of
 2-[2-(4-chlorophenyl)-3-methylbutanoylamino]benzoic acid (I) with
 arylamines. Compound I was prepared by the amidation of anthranilic acid with
 2-(4-chlorophenyl)-3-methylbutanoyl chloride. Antimicrobial activities of
 varying degree was exhibited by all the compds. prepared

RX(1) OF 33 ...A + B ==> C

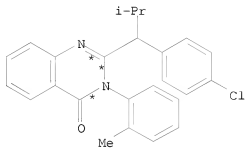
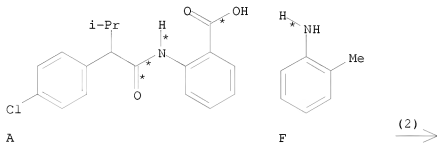


C
 YIELD 75%

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RX(1) RCT A 851191-19-0, B 62-53-3
RGT D 110-86-1 Pyridine
PRO C 851191-03-2
SOL 64-17-5 EtOH
CON 4 hours, reflux
NTE chemoselective

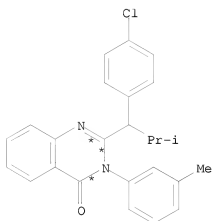
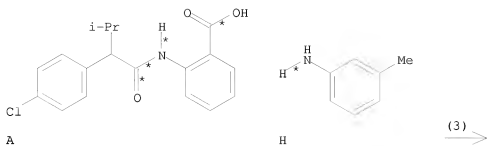
RX(2) OF 33 ...A + F ==> G



YIELD 60%

RX(2) RCT A 851191-19-0, F 95-53-4
RGT D 110-86-1 Pyridine
PRO G 851191-04-3
SOL 64-17-5 EtOH
CON 4 hours, reflux
NTE chemoselective

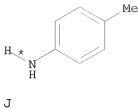
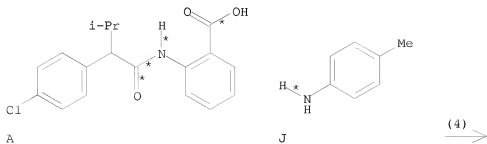
RX(3) OF 33 ...A + H ==> I

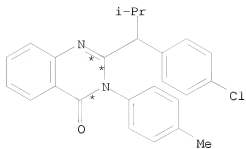


I
YIELD 66%

RX(3) RCT A 851191-19-0, H 108-44-1
RGT D 110-86-1 Pyridine
PRO I 851191-05-4
SOL 64-17-5 EtOH
CON 4 hours, reflux
NTE chemoselective

RX(4) OF 33 ...A + J ==> K

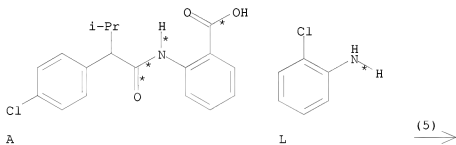




K
YIELD 75%

RX(4) RCT A 851191-19-0, J 106-49-0
RGT D 110-86-1 Pyridine
PRO K 851191-06-5
SOL 64-17-5 EtOH
CON 4 hours, reflux
NTE chemoselective

RX(5) OF 33 ...A + L ==> M



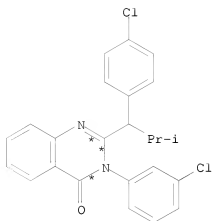
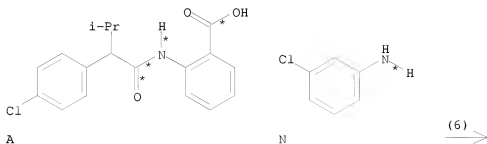
M
YIELD 65%

RX(5) RCT A 851191-19-0, L 95-51-2
RGT D 110-86-1 Pyridine
PRO M 851191-07-6

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SOL 64-17-5 EtOH
CON 4 hours, reflux
NTE chemoselective

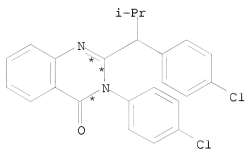
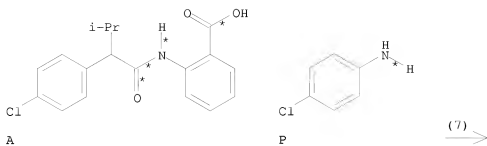
RX(6) OF 33 ...A + N ==> O



O
YIELD 70%

RX(6) RCT A 851191-19-0, N 108-42-9
RGT D 110-86-1 Pyridine
PRO O 851191-08-7
SOL 64-17-5 EtOH
CON 4 hours, reflux
NTE chemoselective

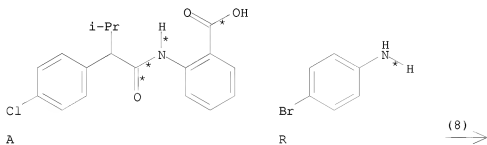
RX(7) OF 33 ...A + P ==> Q

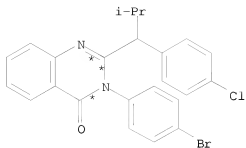


YIELD 68%

RX(7) RCT A 851191-19-0, P 106-47-8
 RGT D 110-86-1 Pyridine
 PRO Q 851191-09-8
 SOL 64-17-5 EtOH
 CON 4 hours, reflux
 NTE chemoselective

RX(8) OF 33 ...A + R ==> S

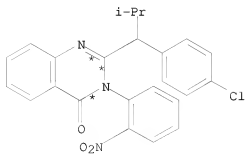
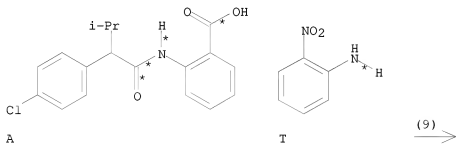




S
YIELD 70%

RX(8) RCT A 851191-19-0, R 106-40-1
RGT D 110-86-1 Pyridine
PRO S 851191-10-1
SOL 64-17-5 EtOH
CON 4 hours, reflux
NTE chemoselective

RX(9) OF 33 ...A + T ==> U



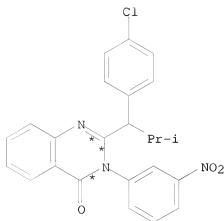
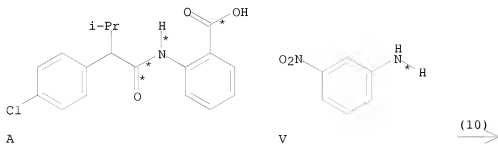
U
YIELD 64%

RX(9) RCT A 851191-19-0, T 88-74-4

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RGT D 110-86-1 Pyridine
 PRO U 851191-11-2
 SOL 64-17-5 EtOH
 CON 4 hours, reflux
 NTE chemoselective

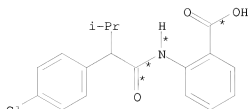
RX(10) OF 33 ...A + V ==> W



W
 YIELD 76%

RX(10) RCT A 851191-19-0, V 99-09-2
 RGT D 110-86-1 Pyridine
 PRO W 851191-12-3
 SOL 64-17-5 EtOH
 CON 4 hours, reflux
 NTE chemoselective

RX(11) OF 33 ...A + X ==> Y

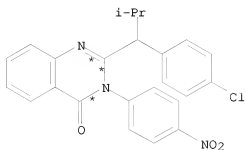


A



X

(11)

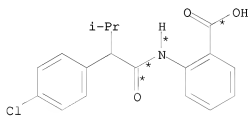


Y

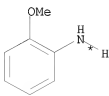
YIELD 72%

RX(11) RCT A 851191-19-0, X 100-01-6
 RGT D 110-86-1 Pyridine
 PRO Y 851191-13-4
 SOL 64-17-5 EtOH
 CON 4 hours, reflux
 NTE chemoselective

RX(12) OF 33 ...A + Z ==> AA

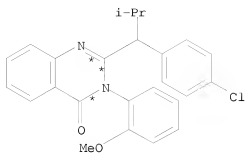


A



Z

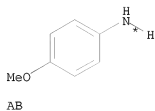
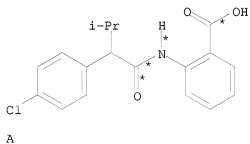
(12)



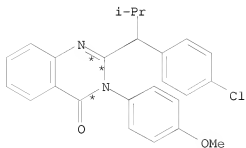
AA
YIELD 80%

RX(12) RCT A 851191-19-0, Z 90-04-0
 RGT D 110-86-1 Pyridine
 PRO AA 851191-14-5
 SOL 64-17-5 EtOH
 CON 4 hours, reflux
 NTE chemoselective

RX(13) OF 33 ...A + AB ==> AC



(13)



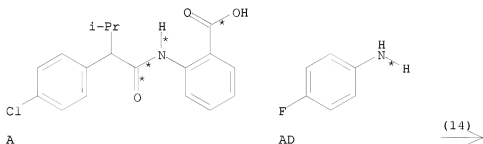
AC
YIELD 78%

RX(13) RCT A 851191-19-0, AB 104-94-9
 RGT D 110-86-1 Pyridine

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PRO AC 851191-15-6
SOL 64-17-5 EtOH
CON 4 hours, reflux
NTE chemoselective

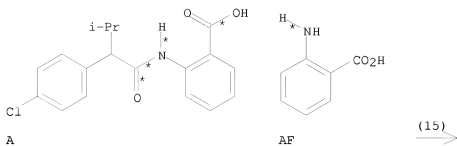
RX(14) OF 33 ...A + AD ==> AE



AE
YIELD 65%

RX(14) RCT A 851191-19-0, AD 371-40-4
RGT D 110-86-1 Pyridine
PRO AE 851191-16-7
SOL 64-17-5 EtOH
CON 4 hours, reflux
NTE chemoselective

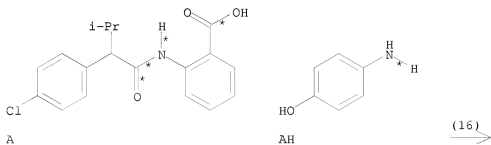
RX(15) OF 33 ...A + AF ==> AG

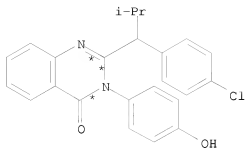


AG
YIELD 60%

RX(15) RCT A 851191-19-0, AF 118-92-3
 RGT D 110-86-1 Pyridine
 PRO AG 851191-17-8
 SOL 64-17-5 EtOH
 CON 4 hours, reflux
 NTE chemoselective

RX(16) OF 33 ...A + AH ==> AI





AI
YIELD 50%

RX(16) RCT A 851191-19-0, AH 123-30-8
RGT D 110-86-1 Pyridine
PRO AI 851191-18-9
SOL 64-17-5 EtOH
CON 4 hours, reflux
NTE chemoselective

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 53 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:430245 CASREACT

TITLE: Synthesis of unsymmetrical
3,3'-biquinazoline-2,2'-diones by condensation of
3-aminoquinazolinones with benzoxazinones; fortuitous
discovery, and further syntheses of
4-H-3-oxa-1,9a,10-triazaanthracen-9-ones

AUTHOR(S): Coogan, Michael P.; Ooi, Li-ling; Pertusati, Fabrizio
CORPORATE SOURCE: Department of Chemistry, Cardiff University, Cardiff,
CF10 3TB, UK

SOURCE: Organic & Biomolecular Chemistry (2005), 3(6),
1134-1139

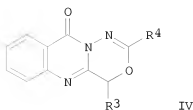
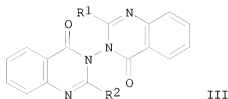
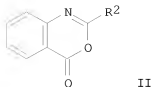
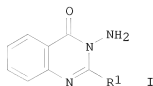
CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

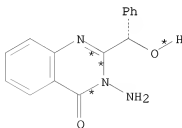
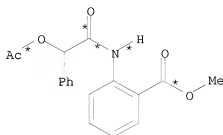
LANGUAGE: English

GI



AB Condensation of 2-alkyl- or 2-aryl-3-aminoquinazolin-4-ones I ($R_1 = \text{EtS}, \text{Me}_3\text{C}, \text{EtO}_2\text{C}, \text{Ph}, \text{PhCH}:\text{CHCH}_2\text{CHMe}$) with benz[1,3]oxazin-4-ones II ($R_2 = \text{H}, \text{Me}, \text{Et}$) gives the unsym. 2,2'-disubstituted 3,3'-biquinazoline-4,4'-diones III. The reaction is tolerant to a range of heteroatom and unsatd. functionality in the quinazolinone 2-position. However, treatment of 3-amino-2-hydroxymethyl-3H-quinazolin-4-ones I ($R_1 = \text{R}_3\text{CHOH}; \text{R}_3 = \text{H}, \text{Me}_2\text{CH}, \text{Ph}$) with benz[1,3]oxazinone II ($R_2 = \text{H}$) at high temps. gave 4H-3-oxa-1,9a,10-triazaanthracen-9-ones IV, an unreported fused heterocyclic system, a more direct synthesis of which by replacement of benzoxazinones with orthoesters $\text{R}_4\text{C}(\text{OEt})_3$ ($\text{R}_4 = \text{H}, \text{Me}, \text{Et}, \text{Ph}$) is presented.

RX(9) OF 21 ...X ==> Y...



(9) \longrightarrow Y
YIELD 64%

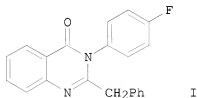
RX(9) RCT X 850870-21-2
RGT Z 302-01-2 N2H4
PRO Y 850870-20-1
SOL 64-17-5 EtOH
CON 5 hours, reflux

REFERENCE COUNT:

19

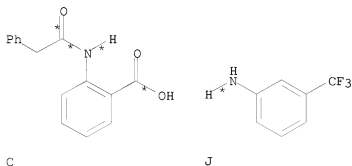
THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

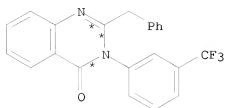
L3 ANSWER 54 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 142:316783 CASREACT
 TITLE: Green chemical multi-component one-pot synthesis of fluorinated 2,3-disubstituted quinazolin-4(3H)-ones under solvent-free conditions and their anti-fungal activity
 AUTHOR(S): Dandia, Anshu; Singh, Ruby; Sarawgi, Pritima
 CORPORATE SOURCE: Department of Chemistry, University of Rajasthan, Jaipur, 302004, India
 SOURCE: Journal of Fluorine Chemistry (2004), 125(12), 1835-1840
 CODEN: JFLCAR; ISSN: 0022-1139
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB A rapid one-pot solvent-free procedure has been developed for the synthesis of fluorinated 2,3-disubstituted quinazolin-4(3H)-ones, e.g., I, by neat three-component cyclocondensation of anthranilic acid, Ph acetyl chloride and substituted anilines under microwave irradiation. The exptl. methodol. and microwave conditions described here are well established, allowing significant rate enhancement and good yields compared to conventional reaction conditions. The reaction is generalized for ortho-, meta-, and para-substituted anilines to give quinazolin-4(3H)-ones. Synthesized compds. have been screened for their antifungal activity.

RX(4) OF 19 ...C + J ==> K





K
YIELD 88%

RX(4) RCT C 28565-98-2

STAGE(1)

RGT F 292600-93-2 KSF (catalyst)

SOL 108-24-7 Ac2O

CON 3 minutes, 141 deg C

STAGE(2)

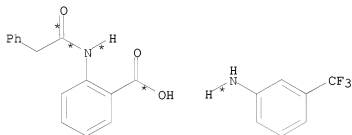
RCT J 98-16-8

CON 7 minutes, 141 deg C

PRO K 848085-19-8

NTE microwave irradiation

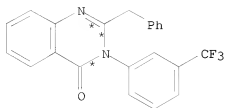
RX(5) OF 19 C + J ==> K



C

J

(5) →



K
YIELD 82%

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RX(5) RCT C 28565-98-2

STAGE(1)

RGT L 1344-28-1 Al2O3

SOL 108-24-7 Ac2O

CON 3 minutes, 132 deg C

STAGE(2)

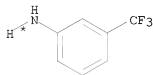
RCT J 98-16-8

CON 10 minutes, 132 deg C

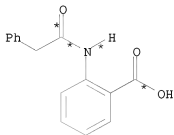
PRO K 848085-19-8

NTE microwave irradiation

RX(7) OF 19 J + C ==> K

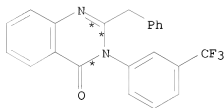


J



C

(7) \longrightarrow



K

YIELD 91%

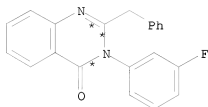
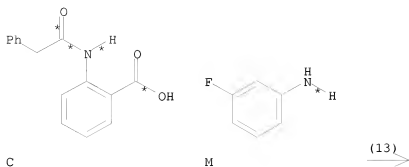
RX(7) RCT J 98-16-8, C 28565-98-2

PRO K 848085-19-8

CON 4 minutes, 164 deg C

NTE microwave irradiation

RX(13) OF 19 ...C + M ==> N



N
YIELD 82%

RX(13) RCT C 28565-98-2

STAGE(1)

RGT F 292600-93-2 KSF (catalyst)

SOL 108-24-7 Ac2O

CON 3 minutes, 142 deg C

STAGE(2)

RGT M 372-19-0

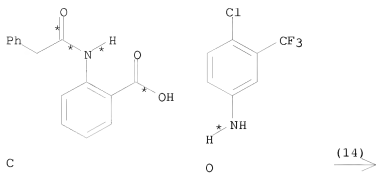
CON 6 minutes, 142 deg C

PRO N 848085-20-1

NTE microwave irradiation

RX(14) OF 19 ...C + O ==> P

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P
YIELD 81%

RX(14) RCT C 28565-98-2

STAGE(1)

RGT F 292600-93-2 KSF (catalyst)

SOL 108-24-7 Ac2O

CON 3 minutes, 137 deg C

STAGE(2)

RCT O 320-51-4

CON 7 minutes, 137 deg C

PRO P 848085-21-2

NTE microwave irradiation

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 55 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

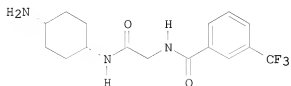
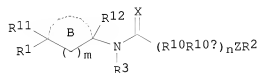
ACCESSION NUMBER: 142:316496 CASREACT

TITLE: Preparation of substituted cycloalkylamine derivatives as modulators of chemokine receptor activity

INVENTOR(S): Carter, Percy H.; Cherney, Robert J.; Batt, Douglas G.; Brown, Gregory D.; Duncia, John V.; Gardner, Daniel S.; Yang, Michael G.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
 SOURCE: PCT Int. Appl., 440 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

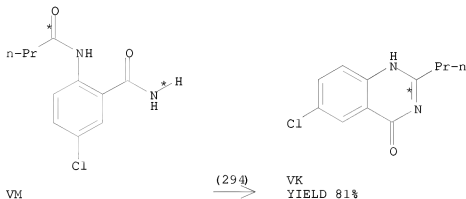
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005020899	A2	20050310	WO 2004-US27195	20040820
WO 2005020899	A3	20050630		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20050054626	A1	20050310	US 2004-923538	20040819
US 7378409	B2	20080527		
EP 1656138	A2	20060517	EP 2004-781805	20040820
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2007502842	T	20070215	JP 2006-524091	20040820
NO 2006000719	A	20060427	NO 2006-719	20060214
PRIORITY APPLN. INFO.:				
			US 2003-496974P	20030821
			US 2004-923538	20040819
			WO 2004-US27195	20040820
OTHER SOURCE(S): MARPAT 142:316496				
GI				



AB Title compds. I [Ring B = saturated or partially unsatd., (un)substituted cycloalkyl or heterocycle; X = O or S; Z = CO, CONR8, NR8, NR8CO, etc.; R1 = H, (un)substituted-alkyl, -alkenyl, -aryl, etc.; R2 = (un)substituted aryl or heteroaryl; R3 = H, Me, or Et; R8 = H, alkyl, or cycloalkyl; R10 and R10a independently = H or (un)substituted alkyl; R11 = H, alkyl, etc.;

R12 = H, alkyl, (un)substituted carbocycle; m = 0-1; n = 1 or 2], or pharmaceutically acceptable salt forms thereof, are prepared and disclosed as modulators of chemokine receptor activity. Thus, e.g., II was prepared by amidation of trans-4-aminocyclohexanol hydrochloride with (3-trifluoromethylbenzoylamino)acetic acid followed by mesylation, substitution with sodium azide and subsequent reduction. I were deemed active (IC50 value of 20 μ M or less) in antagonism of MCP-1 binding to human peripheral blood mononuclear cells. As modulators of MCP-1, I should prove useful for the prevention of asthma, multiple sclerosis, arteriosclerosis, and rheumatoid arthritis.

RX(294) OF 1874 ...VM ==> VK...



RX(294) RCT VM 746671-46-5

STAGE(1)

RGT AU 1310-73-2 NaOH
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 15 minutes, room temperature

STAGE(2)

RGT G 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, pH 2

PRO VK 69729-73-3

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 56 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:240392 CASREACT

TITLE: Synthesis of thieno[2,3-d]pyrimidine and quinazoline derivatives from monothiooxamides

AUTHOR(S): Zavarzin, I. V.; Smirnova, N. G.; Chernoburova, E. I.; Yarovenko, V. N.; Krayushkin, M. M.

CORPORATE SOURCE: N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, 119991, Russia

SOURCE: Russian Chemical Bulletin (Translation of Izvestiya

Akademii Nauk, Seriya Khimicheskaya) (2004), 53(6),
1257-1260

CODEN: RCBUEY; ISSN: 1066-5285

PUBLISHER:

Kluwer Academic/Consultants Bureau

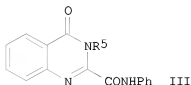
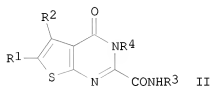
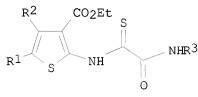
DOCUMENT TYPE:

Journal

LANGUAGE:

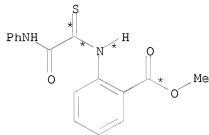
English

GI

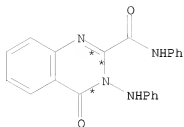


AB A method for syntheses of previously unknown derivs. of thieno[2,3-d]pyrimidines and quinazolines from monothiooxamides is proposed. Thus, heterocyclization of thiophene monothiooxamide derivs. I ($R_1 = \text{Et}$, $R_2 = \text{H}$, $R_3 = \text{H}$, Ph , $\text{C}_6\text{H}_4\text{Cl-4}$; $R_1 = \text{H}$, $R_2 = \text{Ph}$, $R_3 = \text{H}$) with hydrazine or PhCH_2NH_2 gave 45-61% yields of thieno[2,3-d]pyrimidine derivs. II (same R_1 - R_3 ; $R_4 = \text{NH}_2$, CH_2Ph , resp.). Similarly, quinazoline derivs. III ($R_5 = \text{NHPh}$, NH_2 , CH_2Ph) were prepared in 50-74% yields by heterocyclization of the corresponding anthranilic monothiooxamide and PhNHNH_2 , hydrazine or PhCH_2NH_2 , resp.

RX(5) OF 31 ...K + O ==> P



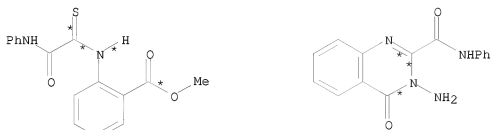
(5) >



P
YIELD 61%

RX(5) RCT K 845298-11-5, O 100-63-0
PRO P 845298-12-6
SOL 64-17-5 EtOH
CON 5 days, reflux

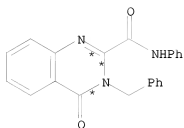
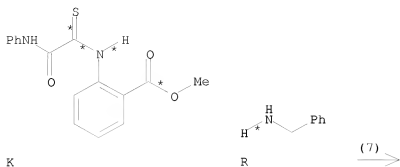
RX(6) OF 31 ...K ==> Q



K (6) Q
YIELD 50%

RX(6) RCT K 845298-11-5
RGT C 302-01-2 N2H4
PRO Q 845298-13-7
SOL 64-17-5 EtOH
CON 3 hours, reflux

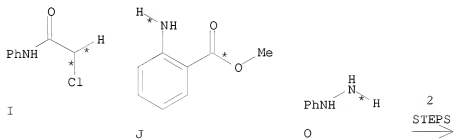
RX(7) OF 31 ...K + R ==> S



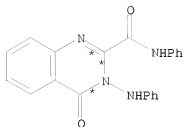
YIELD 75%

RX(7) RCT K 845298-11-5, R 100-46-9
 PRO S 845298-14-8
 SOL 100-46-9 PhCH₂NH₂
 CON 20 minutes, reflux

RX(20) OF 31 COMPOSED OF RX(4), RX(5)
 RX(20) I + J + O \implies P



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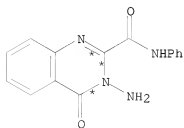
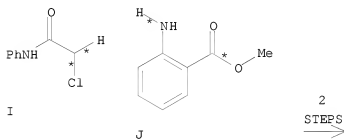


P
YIELD 61%

RX(4) RCT I 587-65-5, J 134-20-3
RGT L 7704-34-9 S, M 121-44-8 Et3N
PRO K 845298-11-5
SOL 68-12-2 DMF
NTE conditions not stated

RX(5) RCT K 845298-11-5, O 100-63-0
PRO P 845298-12-6
SOL 64-17-5 EtOH
CON 5 days, reflux

RX(21) OF 31 COMPOSED OF RX(4), RX(6)
RX(21) I + J ==> Q



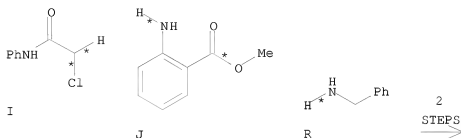
Q
YIELD 50%

RX(4) RCT I 587-65-5, J 134-20-3

RGT L 7704-34-9 S, M 121-44-8 Et3N
 PRO K 845298-11-5
 SOL 68-12-2 DMF
 NTE conditions not stated

RX(6) RCT K 845298-11-5
 RGT C 302-01-2 N2H4
 PRO Q 845298-13-7
 SOL 64-17-5 EtOH
 CON 3 hours, reflux

RX(22) OF 31 COMPOSED OF RX(4), RX(7)
 RX(22) I + J + R ==> S



S
 YIELD 75%

RX(4) RCT I 587-65-5, J 134-20-3
 RGT L 7704-34-9 S, M 121-44-8 Et3N
 PRO K 845298-11-5
 SOL 68-12-2 DMF
 NTE conditions not stated

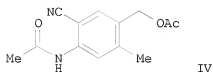
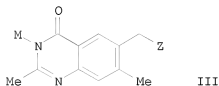
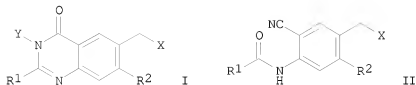
RX(7) RCT K 845298-11-5, R 100-46-9
 PRO S 845298-14-8
 SOL 100-46-9 PhCH2NH2
 CON 20 minutes, reflux

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 57 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 142:198095 CASREACT
 TITLE: A preparation of quinazolin-4-ones via cyclization of
 N-(cyanophenyl)acetamide derivatives
 INVENTOR(S): Godfrey, Andrew Aydon
 PATENT ASSIGNEE(S): BTG International Limited, UK
 SOURCE: PCT Int. Appl., 29 pp.
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 PATENT INFORMATION:

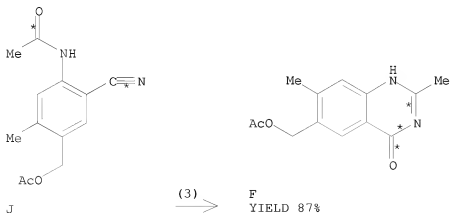
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005012260	A2	20050210	WO 2004-GB3141	20040720
WO 2005012260	A3	20050407		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2004261453	A1	20050210	AU 2004-261453	20040720
CA 2531750	A1	20050210	CA 2004-2531750	20040720
EP 1675831	A2	20060705	EP 2004-743476	20040720
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK			
JP 2007500175	T	20070111	JP 2006-521644	20040720
US 20060189804	A1	20060824	US 2005-562112	20051223
IN 2006DN00057	A	20070824	IN 2006-DN57	20060103
MX 2006000883	A	20060419	MX 2006-883	20060123
KR 2006056962	A	20060525	KR 2006-701909	20060127
PRIORITY APPLN. INFO.:			GB 2003-17631	20030728
			WO 2004-GB3141	20040720

OTHER SOURCE(S): MARPAT 142:198095
 GI



AB The invention relates to a preparation of quinazolin-4-one derivs. of formula I [wherein: R1 and R2 are independently H or Me; Y is a protecting group; X is a leaving group], useful as intermediates in preparation of antitumor agents. The invention compds. I were prepared via cyclization of amides of formula II. For instance, quinazolin-4-one derivative III(HBr (Z = Br, M = H) was prepared via intramol. cyclization of N-(cyanophenyl)acetamide derivative IV, N-protection of the obtained quinazoline derivative III (Z = OAc; M = H) by chloromethyl pivalate, and subsequent bromination (yields: cyclization - 87%, bromination - 89%).

RX(3) OF 45 . . . J ==> F . . .

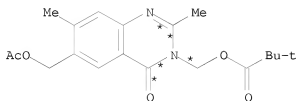
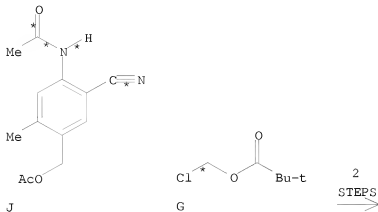


RX(3) RCT J 838858-87-0
 RGT K 7647-01-0 HC1

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PRO F 838858-86-9
SOL 67-63-0 Me2CHOH
CON SUBSTAGE(1) 60 minutes
SUBSTAGE(2) 30 deg C
NTE HCl gas used

RX(12) OF 45 COMPOSED OF RX(3), RX(2)
RX(12) J + G ==> A



A
YIELD 62%

RX(3) RCT J 838858-87-0
RGT K 7647-01-0 HCl
PRO F 838858-86-9
SOL 67-63-0 Me2CHOH
CON SUBSTAGE(1) 60 minutes
SUBSTAGE(2) 30 deg C
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)
RGT H 584-08-7 K2CO3
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 16 hours, 50 deg C

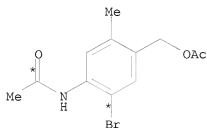
STAGE(2)
RCT G 18997-19-8

10/ 562,112

CON SUBSTAGE(1) 2.5 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(13) OF 45 COMPOSED OF RX(4), RX(3)
RX(13) M + N ==> F

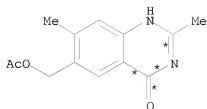


M



N

2
STEPS
→



F
YIELD 87%

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0

RGT K 7647-01-0 HCl

PRO F 838858-86-9

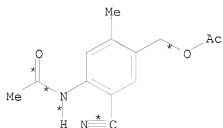
SOL 67-63-0 Me2CHOH

CON SUBSTAGE(1) 60 minutes

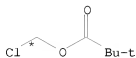
SUBSTAGE(2) 30 deg C

NTE HCl gas used

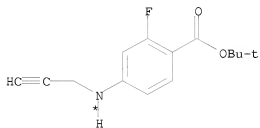
RX(21) OF 45 COMPOSED OF RX(3), RX(2), RX(1), RX(9)
 RX(21) J + G + AI ==> AG



J

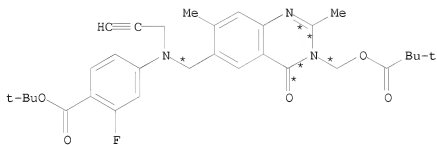


G



AI

4
 STEPS
 →



AG

YIELD 80%

RX(3) RCT J 838858-87-0
 RGT K 7647-01-0 HCl
 PRO F 838858-86-9
 SOL 67-63-0 Me2CHOH
 CON SUBSTAGE(1) 60 minutes
 SUBSTAGE(2) 30 deg C
 NTE HCl gas used

RX(2) RCT F 838858-86-9

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STAGE(1)
  RGT  H 584-08-7 K2CO3
  SOL  67-68-5 DMSO
  CON  SUBSTAGE(1) 50 deg C
        SUBSTAGE(2) 16 hours, 50 deg C

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STAGE(2)
  RGT  G 18997-19-8
  CON  SUBSTAGE(1) 2.5 hours, 50 deg C
        SUBSTAGE(2) 30 minutes, 50 deg C

```

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

```

STAGE(1)
  RGT  C 10035-10-6 HBr
  SOL  7732-18-5 Water, 64-19-7 AcOH
  CON  SUBSTAGE(1) room temperature
        SUBSTAGE(2) room temperature -> 60 deg C

```

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STAGE(2)
  RGT  C 10035-10-6 HBr
  SOL  7732-18-5 Water, 64-19-7 AcOH
  CON  SUBSTAGE(1) 2 hours, 60 deg C
        SUBSTAGE(2) 3 hours, 60 deg C
        SUBSTAGE(3) 60 deg C -> 16 deg C
        SUBSTAGE(4) 18 hours, 16 deg C

```

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

```

STAGE(1)
  RGT  AJ 144-55-8 NaHCO3
  SOL  7732-18-5 Water, 108-88-3 PhMe
  CON  SUBSTAGE(1) 30 minutes, 65 deg C
        SUBSTAGE(2) 1 hour

```

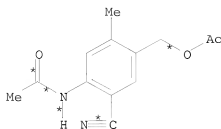
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STAGE(2)
  RCT  AI 140373-03-1
  RGT  AK 108-48-5 2,6-Lutidine
  SOL  108-88-3 PhMe
  CON  SUBSTAGE(1) 105 deg C
        SUBSTAGE(2) 24 hours, 105 deg C
        SUBSTAGE(3) 105 deg C -> 65 deg C

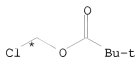
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PRO AG 153538-14-8

RX(22) OF 45 COMPOSED OF RX(3), RX(2), RX(1)
 RX(22) J + G ==> B

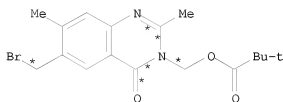


J



G

3
STEPS
→



● HBr

B

YIELD 89%

RX(3) RCT J 838858-87-0
 RGT K 7647-01-0 HCl
 PRO F 838858-86-9
 SOL 67-63-0 Me2CHOH
 CON SUBSTAGE(1) 60 minutes
 SUBSTAGE(2) 30 deg C
 NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)

RGT H 584-08-7 K2CO3
 SOL 67-68-5 DMSO
 CON SUBSTAGE(1) 50 deg C
 SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)

RCT G 18997-19-8
 CON SUBSTAGE(1) 2.5 hours, 50 deg C
 SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)

RGT C 10035-10-6 HBr

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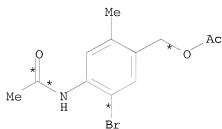
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)

RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) 2 hours, 60 deg C
SUBSTAGE(2) 3 hours, 60 deg C
SUBSTAGE(3) 60 deg C -> 16 deg C
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

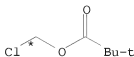
RX(23) OF 45 COMPOSED OF RX(4), RX(3), RX(2), RX(1)
RX(23) M + N + G ==> B



M

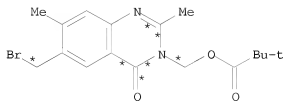


N



G

4
STEPS
→



● HBr

B
YIELD 89%

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF
CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3)

RCT J 838858-87-0

RGT K 7647-01-0 HCl

PRO F 838858-86-9

SOL 67-63-0 Me2CHOH

CON SUBSTAGE(1) 60 minutes

SUBSTAGE(2) 30 deg C

NTE HCl gas used

RX(2)

RCT F 838858-86-9

STAGE(1)

RGT H 584-08-7 K2CO3

SOL 67-68-5 DMSO

CON SUBSTAGE(1) 50 deg C

SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)

RCT G 18997-19-8

CON SUBSTAGE(1) 2.5 hours, 50 deg C

SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1)

RCT A 838858-85-8

STAGE(1)

RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)

RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) 2 hours, 60 deg C

SUBSTAGE(2) 3 hours, 60 deg C

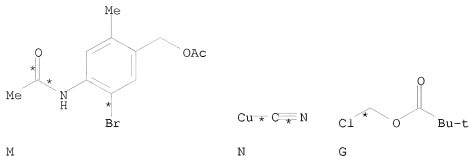
SUBSTAGE(3) 60 deg C -> 16 deg C

SUBSTAGE(4) 18 hours, 16 deg C

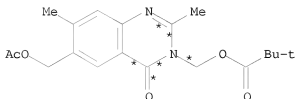
PRO B 838858-84-7

RX(24) OF 45 COMPOSED OF RX(4), RX(3), RX(2)

RX(24) M + N + G ==> A



3
STEPS
→



A
YIELD 62%

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3)

RCT J 838858-87-0

RGT K 7647-01-0 HCl

PRO F 838858-86-9

SOL 67-63-0 Me2CHOH

CON SUBSTAGE(1) 60 minutes

SUBSTAGE(2) 30 deg C

NTE HCl gas used

RX(2)

RCT F 838858-86-9

STAGE(1)

RGT H 584-08-7 K2CO3

SOL 67-68-5 DMSO

CON SUBSTAGE(1) 50 deg C

SUBSTAGE(2) 16 hours, 50 deg C

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STAGE(2)

RCT G 18997-19-8

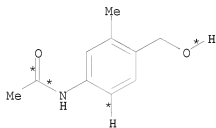
CON SUBSTAGE(1) 2.5 hours, 50 deg C

SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(25) OF 45 COMPOSED OF RX(5), RX(4), RX(3), RX(2)

RX(25) Q + R + N + G ==> A



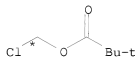
Q



R

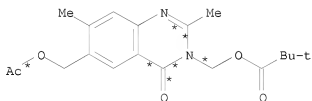


N



G

4
STEPS
→



A

YIELD 62%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et3N

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RCT R 75-36-5

CON SUBSTAGE(1) 2 hours, 50 deg C


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                SUBSTAGE(2) 30 minutes, 50 deg C
                SUBSTAGE(3) 50 deg C -> 20 deg C

    STAGE(3)
        RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,
            5-(bromomethyl)-1,2,3,4,7,7-hexachloro-
        SOL 75-05-8 MeCN
        CON SUBSTAGE(1) 50 deg C
            SUBSTAGE(2) 60 minutes
            SUBSTAGE(3) 50 deg C -> 20 deg C

    PRO M 838858-88-1
    NTE regioselective

RX(4)    RCT M 838858-88-1, N 544-92-3

        STAGE(1)
            SOL 68-12-2 DMF
            CON SUBSTAGE(1) 6 hours, 90 deg C
                SUBSTAGE(2) 90 deg C -> 60 deg C

        STAGE(2)
            RGT O 7440-66-6 Zn
            CON SUBSTAGE(1) 60 deg C
                SUBSTAGE(2) 60 deg C -> 90 deg C

    PRO J 838858-87-0
    NTE inert, incremental addition of reagent in second stage

RX(3)    RCT J 838858-87-0
        RGT K 7647-01-0 HCl
        PRO F 838858-86-9
        SOL 67-63-0 Me2CHOH
        CON SUBSTAGE(1) 60 minutes
            SUBSTAGE(2) 30 deg C
        NTE HCl gas used

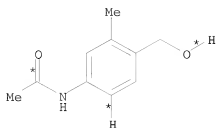
RX(2)    RCT F 838858-86-9

        STAGE(1)
            RGT H 584-08-7 K2CO3
            SOL 67-68-5 DMSO
            CON SUBSTAGE(1) 50 deg C
                SUBSTAGE(2) 16 hours, 50 deg C

        STAGE(2)
            RCT G 18997-19-8
            CON SUBSTAGE(1) 2.5 hours, 50 deg C
                SUBSTAGE(2) 30 minutes, 50 deg C

    PRO A 838858-85-8

RX(26) OF 45 COMPOSED OF RX(5), RX(4), RX(3)
RX(26)    Q + R + N ==> F
```



Q

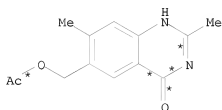


R



N

3
STEPS
→



F
YIELD 87%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et3N

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RCT R 75-36-5

CON SUBSTAGE(1) 2 hours, 50 deg C

SUBSTAGE(2) 30 minutes, 50 deg C

SUBSTAGE(3) 50 deg C -> 20 deg C

STAGE(3)

RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,
5-(bromomethyl)-1,2,3,4,7,7-hexachloro-

SOL 75-05-8 MeCN

CON SUBSTAGE(1) 50 deg C

SUBSTAGE(2) 60 minutes

SUBSTAGE(3) 50 deg C -> 20 deg C

PRO M 838858-88-1

NTE regioselective

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3)

RCT J 838858-87-0

RGT K 7647-01-0 HCl

PRO F 838858-86-9

SOL 67-63-0 Me2CHOH

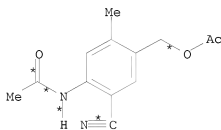
CON SUBSTAGE(1) 60 minutes

SUBSTAGE(2) 30 deg C

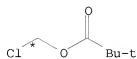
NTE HCl gas used

RX(34) OF 45 COMPOSED OF RX(3), RX(2), RX(1), RX(9), RX(8), RX(7), RX(6)

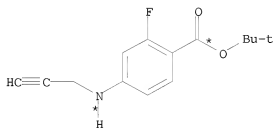
RX(34) J + G + AI + AC ==> X



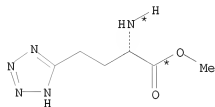
J



G



AI

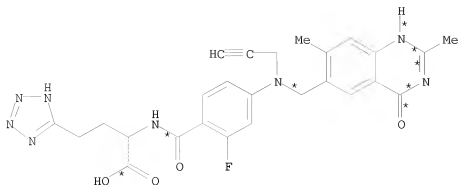


AC

7

STEPS





X

YIELD 92%

RX(3) RCT J 838858-87-0
 RGT K 7647-01-0 HCl
 PRO F 838858-86-9
 SOL 67-63-0 Me2CHOH
 CON SUBSTAGE(1) 60 minutes
 SUBSTAGE(2) 30 deg C
 NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)

RGT H 584-08-7 K2CO3
 SOL 67-68-5 DMSO
 CON SUBSTAGE(1) 50 deg C
 SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)

RCT G 18997-19-8
 CON SUBSTAGE(1) 2.5 hours, 50 deg C
 SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)

RGT C 10035-10-6 HBr
 SOL 7732-18-5 Water, 64-19-7 AcOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)

RGT C 10035-10-6 HBr
 SOL 7732-18-5 Water, 64-19-7 AcOH
 CON SUBSTAGE(1) 2 hours, 60 deg C
 SUBSTAGE(2) 3 hours, 60 deg C
 SUBSTAGE(3) 60 deg C -> 16 deg C
 SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)

RGT AJ 144-55-8 NaHCO₃

SOL 7732-18-5 Water, 108-88-3 PhMe

CON SUBSTAGE(1) 30 minutes, 65 deg C

SUBSTAGE(2) 1 hour

STAGE(2)

RCT AI 140373-03-1

RGT AK 108-48-5 2,6-Lutidine

SOL 108-88-3 PhMe

CON SUBSTAGE(1) 105 deg C

SUBSTAGE(2) 24 hours, 105 deg C

SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)

RGT AH 64-18-6 HCO₂H

SOL 7732-18-5 Water

CON 5 hours, 40 deg C

STAGE(2)

RGT D 7732-18-5 Water

CON 3 hours

PRO AB 140373-09-7

RX(7) RCT AB 140373-09-7

STAGE(1)

RGT AD 7719-09-7 SOCl₂SOL 75-09-2 CH₂Cl₂

CON SUBSTAGE(1) 30 minutes, 10 deg C

SUBSTAGE(2) 10 deg C -> 20 deg C

STAGE(2)

RCT AC 127105-49-1

RGT AE 7087-68-5 EtN(Pr-i)₂SOL 75-09-2 CH₂Cl₂

CON SUBSTAGE(1) 3 hours, 10 deg C

SUBSTAGE(2) 16 hours

STAGE(3)

RGT E 64-19-7 AcOH

PRO W 247904-63-8

NIE inert

RX(6) RCT W 247904-63-8

STAGE(1)

RGT Y 1310-73-2 NaOH

SOL 7732-18-5 Water, 109-99-9 THF

CON SUBSTAGE(1) 15 deg C

SUBSTAGE(2) 15 deg C -> 24 deg C

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SUBSTAGE(3) 19 hours, 24 deg C

STAGE(2)

RGT Z 7631-90-5 NaHSO3

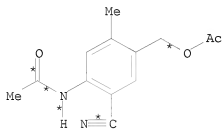
SOL 7732-18-5 Water

CON 40 minutes, 24 deg C

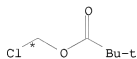
PRO X 153537-73-6

RX(35) OF 45 COMPOSED OF RX(3), RX(2), RX(1), RX(9), RX(8), RX(7)

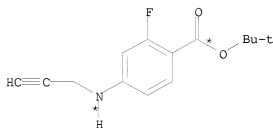
RX(35) J + G + AI + AC ==> W



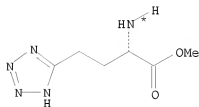
J



G



AI

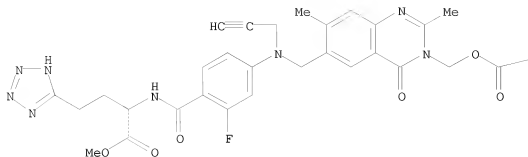


AC

6

STEPS





— Bu-t

W
YIELD 82%

RX(3) RCT J 838858-87-0
RGT K 7647-01-0 HCl
PRO F 838858-86-9
SOL 67-63-0 Me2CHOH
CON SUBSTAGE(1) 60 minutes
SUBSTAGE(2) 30 deg C
NTE HCl gas used

RX(2) RCT F 838858-86-9
STAGE(1)
RGT H 584-08-7 K2CO3
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)
RCT G 18997-19-8
CON SUBSTAGE(1) 2.5 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8
STAGE(1)
RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)
RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) 2 hours, 60 deg C
SUBSTAGE(2) 3 hours, 60 deg C
SUBSTAGE(3) 60 deg C -> 16 deg C
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)
RGT AJ 144-55-8 NaHCO3
SOL 7732-18-5 Water, 108-88-3 PhMe
CON SUBSTAGE(1) 30 minutes, 65 deg C
SUBSTAGE(2) 1 hour

STAGE(2)
RCT AI 140373-03-1
RGT AK 108-48-5 2,6-Lutidine
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 105 deg C
SUBSTAGE(2) 24 hours, 105 deg C
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)
RGT AH 64-18-6 HCO2H
SOL 7732-18-5 Water
CON 5 hours, 40 deg C

STAGE(2)
RGT D 7732-18-5 Water
CON 3 hours

PRO AB 140373-09-7

RX(7) RCT AB 140373-09-7

STAGE(1)
RGT AD 7719-09-7 SOCl2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 30 minutes, 10 deg C
SUBSTAGE(2) 10 deg C -> 20 deg C

STAGE(2)
RCT AC 127105-49-1
RGT AE 7087-68-5 EtN(Pr-i)2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 3 hours, 10 deg C
SUBSTAGE(2) 16 hours

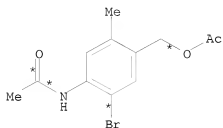
STAGE(3)
RGT E 64-19-7 AcOH

PRO W 247904-63-8

NTE inert

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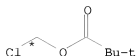
RX(36) OF 45 COMPOSED OF RX(4), RX(3), RX(2), RX(1), RX(9), RX(8), RX(7), RX(6)
 RX(36) M + N + G + AI + AC ==> X



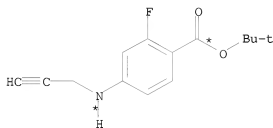
M



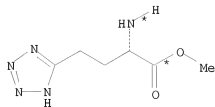
N



G

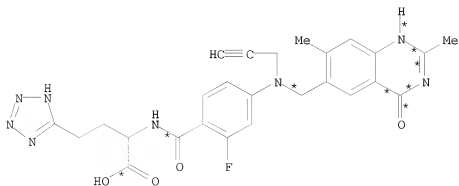


AI



AC

8
 STEPS
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X

YIELD 92%

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)
SOL 68-12-2 DMF
CON SUBSTAGE(1) 6 hours, 90 deg C
SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)
RGT O 7440-66-6 Zn
CON SUBSTAGE(1) 60 deg C
SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0
NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0
RGT K 7647-01-0 HCl
PRO F 838858-86-9
SOL 67-63-0 Me2CHOH
CON SUBSTAGE(1) 60 minutes
SUBSTAGE(2) 30 deg C
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)
RGT H 584-08-7 K2CO3
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)
RCT G 18997-19-8
CON SUBSTAGE(1) 2.5 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)
RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)
RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) 2 hours, 60 deg C
SUBSTAGE(2) 3 hours, 60 deg C
SUBSTAGE(3) 60 deg C -> 16 deg C
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)
RGT AJ 144-55-8 NaHCO3
SOL 7732-18-5 Water, 108-88-3 PhMe

CON SUBSTAGE(1) 30 minutes, 65 deg C
SUBSTAGE(2) 1 hour

STAGE(2)

RCT AI 140373-03-1
RGT AK 108-48-5 2,6-Lutidine
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 105 deg C
SUBSTAGE(2) 24 hours, 105 deg C
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)

RGT AH 64-18-6 HCO₂H
SOL 7732-18-5 Water
CON 5 hours, 40 deg C

STAGE(2)

RGT D 7732-18-5 Water
CON 3 hours

PRO AB 140373-09-7

RX(7) RCT AB 140373-09-7

STAGE(1)

RGT AD 7719-09-7 SOCl₂
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 30 minutes, 10 deg C
SUBSTAGE(2) 10 deg C -> 20 deg C

STAGE(2)

RCT AC 127105-49-1
RGT AE 7087-68-5 EtN(Pr-i)₂
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 3 hours, 10 deg C
SUBSTAGE(2) 16 hours

STAGE(3)

RGT E 64-19-7 AcOH

PRO W 247904-63-8

NTE inert

RX(6) RCT W 247904-63-8

STAGE(1)

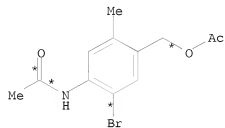
RGT Y 1310-73-2 NaOH
SOL 7732-18-5 Water, 109-99-9 THF
CON SUBSTAGE(1) 15 deg C
SUBSTAGE(2) 15 deg C -> 24 deg C
SUBSTAGE(3) 19 hours, 24 deg C

STAGE(2)

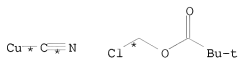
RGT Z 7631-90-5 NaHSO₃
SOL 7732-18-5 Water
CON 40 minutes, 24 deg C

PRO X 153537-73-6

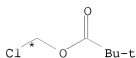
RX(37) OF 45 COMPOSED OF RX(4), RX(3), RX(2), RX(1), RX(9), RX(8), RX(7)
 RX(37) M + N + G + AI + AC ==> W



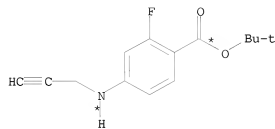
M



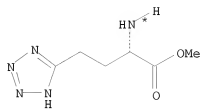
N



G



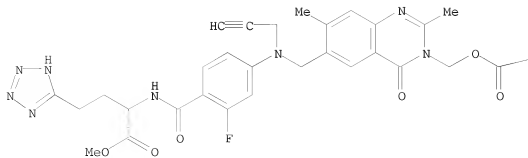
AI



AC

7
 STEPS
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PAGE 1-A



Bu-t

W
YIELD 82%

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0

RGT K 7647-01-0 HCl

PRO F 838858-86-9

SOL 67-63-0 Me2CHOH

CON SUBSTAGE(1) 60 minutes

SUBSTAGE(2) 30 deg C

NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)

RGT H 584-08-7 K2CO3

SOL 67-68-5 DMSO

CON SUBSTAGE(1) 50 deg C

SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)

RGT G 18997-19-8

CON SUBSTAGE(1) 2.5 hours, 50 deg C

SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)

RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)

RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) 2 hours, 60 deg C
SUBSTAGE(2) 3 hours, 60 deg C
SUBSTAGE(3) 60 deg C -> 16 deg C
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)
RGT AJ 144-55-8 NaHCO3
SOL 7732-18-5 Water, 108-88-3 PhMe
CON SUBSTAGE(1) 30 minutes, 65 deg C
SUBSTAGE(2) 1 hour

STAGE(2)
RCT AI 140373-03-1
RGT AK 108-48-5 2,6-Lutidine
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 105 deg C
SUBSTAGE(2) 24 hours, 105 deg C
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)
RGT AH 64-18-6 HCO2H
SOL 7732-18-5 Water
CON 5 hours, 40 deg C

STAGE(2)
RGT D 7732-18-5 Water
CON 3 hours

PRO AB 140373-09-7

RX(7) RCT AB 140373-09-7

STAGE(1)
RGT AD 7719-09-7 SOCl2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 30 minutes, 10 deg C
SUBSTAGE(2) 10 deg C -> 20 deg C

STAGE(2)
RCT AC 127105-49-1
RGT AE 7087-68-5 EtN(Pr-i)2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 3 hours, 10 deg C
SUBSTAGE(2) 16 hours

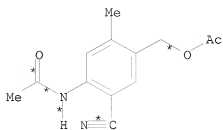
STAGE(3)
RGT E 64-19-7 AcOH

PRO W 247904-63-8

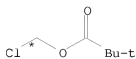
NTE inert

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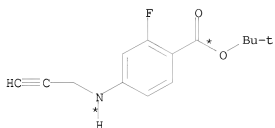
RX(38) OF 45 COMPOSED OF RX(3), RX(2), RX(1), RX(9), RX(8)
 RX(38) J + G + AI ==> AB



J

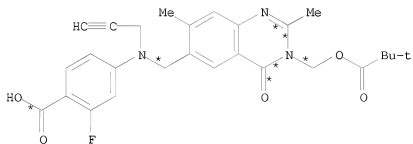


G



AI

5
STEPS
→



AB

YIELD 98%

RX(3) RCT J 838858-87-0
 RGT K 7647-01-0 HCl
 PRO F 838858-86-9
 SOL 67-63-0 Me2CHOH
 CON SUBSTAGE(1) 60 minutes
 SUBSTAGE(2) 30 deg C
 NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)
RGT H 584-08-7 K2CO3
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)
RCT G 18997-19-8
CON SUBSTAGE(1) 2.5 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)
RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)
RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) 2 hours, 60 deg C
SUBSTAGE(2) 3 hours, 60 deg C
SUBSTAGE(3) 60 deg C -> 16 deg C
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)
RGT AJ 144-55-8 NaHCO3
SOL 7732-18-5 Water, 108-88-3 PhMe
CON SUBSTAGE(1) 30 minutes, 65 deg C
SUBSTAGE(2) 1 hour

STAGE(2)
RCT AI 140373-03-1
RGT AK 108-48-5 2,6-Lutidine
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 105 deg C
SUBSTAGE(2) 24 hours, 105 deg C
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

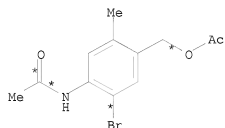
STAGE(1)
RGT AH 64-18-6 HCO2H
SOL 7732-18-5 Water
CON 5 hours, 40 deg C

STAGE(2)
RGT D 7732-18-5 Water
CON 3 hours

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PRO AB 140373-09-7

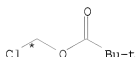
RX(39) OF 45 COMPOSED OF RX(4), RX(3), RX(2), RX(1), RX(9), RX(8)
 RX(39) M + N + G + AI ==> AB



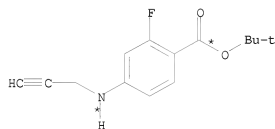
M



N

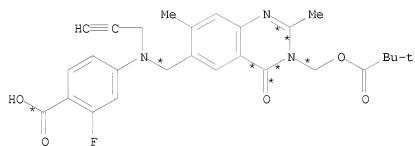


G



AI

6
 STEPS
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AB

YIELD 98%

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)
RGT O 7440-66-6 Zn
CON SUBSTAGE(1) 60 deg C
SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0
NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0
RGT K 7647-01-0 HCl
PRO F 838858-86-9
SOL 67-63-0 Me2CHOH
CON SUBSTAGE(1) 60 minutes
SUBSTAGE(2) 30 deg C
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)
RGT H 584-08-7 K2CO3
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)
RCT G 18997-19-8
CON SUBSTAGE(1) 2.5 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)
RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)
RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) 2 hours, 60 deg C
SUBSTAGE(2) 3 hours, 60 deg C
SUBSTAGE(3) 60 deg C -> 16 deg C
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)
RGT AJ 144-55-8 NaHCO3
SOL 7732-18-5 Water, 108-88-3 PhMe
CON SUBSTAGE(1) 30 minutes, 65 deg C
SUBSTAGE(2) 1 hour

STAGE(2)
RCT AI 140373-03-1
RGT AK 108-48-5 2,6-Lutidine

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SOL 108-88-3 PhMe
 CON SUBSTAGE(1) 105 deg C
 SUBSTAGE(2) 24 hours, 105 deg C
 SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

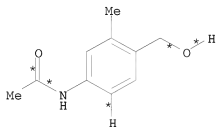
STAGE(1)
 RGT AH 64-18-6 HCO2H
 SOL 7732-18-5 Water
 CON 5 hours, 40 deg C

STAGE(2)
 RGT D 7732-18-5 Water
 CON 3 hours

PRO AB 140373-09-7

RX(40) OF 45 COMPOSED OF RX(5), RX(4), RX(3), RX(2), RX(1), RX(9), RX(8)

RX(40) Q + R + N + G + AI ==> AB



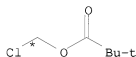
Q



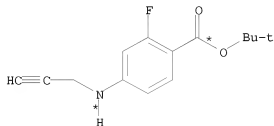
R



N

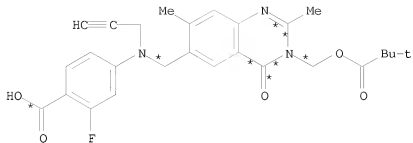


G



AI

7
 STEPS
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AB
YIELD 98%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et3N
SOL 141-78-6 AcOEt
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RCT R 75-36-5
CON SUBSTAGE(1) 2 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C
SUBSTAGE(3) 50 deg C -> 20 deg C

STAGE(3)

RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,
5-(bromomethyl)-1,2,3,4,7,7-hexachloro-
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 60 minutes
SUBSTAGE(3) 50 deg C -> 20 deg C

PRO M 838858-88-1
NTE regioselective

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF
CON SUBSTAGE(1) 6 hours, 90 deg C
SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn
CON SUBSTAGE(1) 60 deg C
SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0
NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0
RGT K 7647-01-0 HCl
PRO F 838858-86-9

SOL 67-63-0 Me2CHOH
CON SUBSTAGE(1) 60 minutes
SUBSTAGE(2) 30 deg C
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)
RGT H 584-08-7 K2CO3
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)
RCT G 18997-19-8
CON SUBSTAGE(1) 2.5 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)
RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)
RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) 2 hours, 60 deg C
SUBSTAGE(2) 3 hours, 60 deg C
SUBSTAGE(3) 60 deg C -> 16 deg C
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)
RGT AJ 144-55-8 NaHCO3
SOL 7732-18-5 Water, 108-88-3 PhMe
CON SUBSTAGE(1) 30 minutes, 65 deg C
SUBSTAGE(2) 1 hour

STAGE(2)
RCT AI 140373-03-1
RGT AK 108-48-5 2,6-Lutidine
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 105 deg C
SUBSTAGE(2) 24 hours, 105 deg C
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)
RGT AH 64-18-6 HCO2H

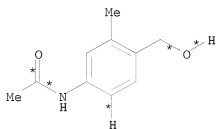
10/ 562,112

SOL 7732-18-5 Water
CON 5 hours, 40 deg C

STAGE(2)
RGT D 7732-18-5 Water
CON 3 hours

PRO AB 140373-09-7

RX(41) OF 45 COMPOSED OF RX(5), RX(4), RX(3), RX(2), RX(1), RX(9), RX(8), RX(7)
RX(41) Q + R + N + G + AI + AC ==> W



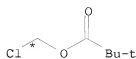
Q



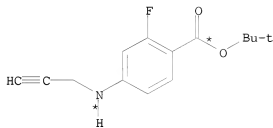
R



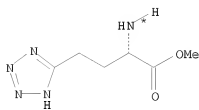
N



G

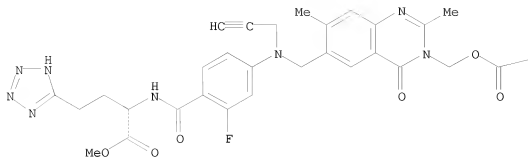


AI



AC

8
STEPS
→



— Bu-t

W
YIELD 82%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et3N
SOL 141-78-6 AcOEt
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RCT R 75-36-5
CON SUBSTAGE(1) 2 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C
SUBSTAGE(3) 50 deg C -> 20 deg C

STAGE(3)

RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,
5-(bromomethyl)-1,2,3,4,7,7-hexachloro-
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 60 minutes
SUBSTAGE(3) 50 deg C -> 20 deg C

PRO M 838858-88-1
NTE regioselective

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF
CON SUBSTAGE(1) 6 hours, 90 deg C
SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn
CON SUBSTAGE(1) 60 deg C
SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0
NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0
RGT K 7647-01-0 HCl
PRO F 838858-86-9
SOL 67-63-0 Me2CHOH
CON SUBSTAGE(1) 60 minutes
SUBSTAGE(2) 30 deg C
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)
RGT H 584-08-7 K2CO3
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)
RCT G 18997-19-8
CON SUBSTAGE(1) 2.5 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)
RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)
RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) 2 hours, 60 deg C
SUBSTAGE(2) 3 hours, 60 deg C
SUBSTAGE(3) 60 deg C -> 16 deg C
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)
RGT AJ 144-55-8 NaHCO3
SOL 7732-18-5 Water, 108-88-3 PhMe
CON SUBSTAGE(1) 30 minutes, 65 deg C
SUBSTAGE(2) 1 hour

STAGE(2)
RCT AI 140373-03-1
RGT AK 108-48-5 2,6-Lutidine
SOL 108-88-3 PhMe

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CON SUBSTAGE(1) 105 deg C
SUBSTAGE(2) 24 hours, 105 deg C
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)
RGT AH 64-18-6 HCO2H
SOL 7732-18-5 Water
CON 5 hours, 40 deg C

STAGE(2)
RGT D 7732-18-5 Water
CON 3 hours

PRO AB 140373-09-7

RX(7) RCT AB 140373-09-7

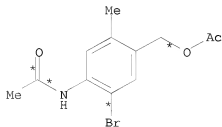
STAGE(1)
RGT AD 7719-09-7 SOC12
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 30 minutes, 10 deg C
SUBSTAGE(2) 10 deg C -> 20 deg C

STAGE(2)
RCT AC 127105-49-1
RGT AE 7087-68-5 EtN(Pr-i)2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 3 hours, 10 deg C
SUBSTAGE(2) 16 hours

STAGE(3)
RGT E 64-19-7 AcOH

PRO W 247904-63-8
NTE inert

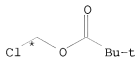
RX(42) OF 45 COMPOSED OF RX(4), RX(3), RX(2), RX(1), RX(9)
RX(42) M + N + G + AI ==> AG



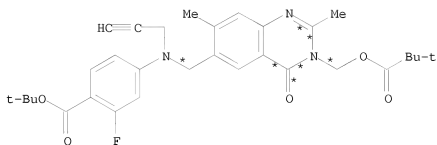
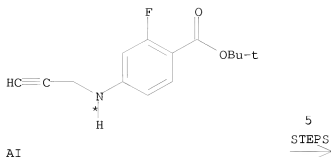
M



N



G



RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 6 hours, 90 deg C

SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn

CON SUBSTAGE(1) 60 deg C

SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0

NTE inert, incremental addition of reagent in second stage

RX(3)

RCT J 838858-87-0

RGT K 7647-01-0 HCl

PRO F 838858-86-9

SOL 67-63-0 Me2CHOH

CON SUBSTAGE(1) 60 minutes

SUBSTAGE(2) 30 deg C

NTE HCl gas used

RX(2)

RCT F 838858-86-9

STAGE(1)

RGT H 584-08-7 K2CO3

SOL 67-68-5 DMSO

CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)

RCT G 18997-19-8

CON SUBSTAGE(1) 2.5 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)

RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)

RGT C 10035-10-6 HBr

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) 2 hours, 60 deg C
SUBSTAGE(2) 3 hours, 60 deg C
SUBSTAGE(3) 60 deg C -> 16 deg C
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)

RGT AJ 144-55-8 NaHCO3

SOL 7732-18-5 Water, 108-88-3 PhMe

CON SUBSTAGE(1) 30 minutes, 65 deg C
SUBSTAGE(2) 1 hour

STAGE(2)

RCT AI 140373-03-1

RGT AK 108-48-5 2,6-Lutidine

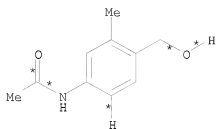
SOL 108-88-3 PhMe

CON SUBSTAGE(1) 105 deg C
SUBSTAGE(2) 24 hours, 105 deg C
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(43) OF 45 COMPOSED OF RX(5), RX(4), RX(3), RX(2), RX(1), RX(9)
RX(43) Q + R + N + G + AI ==> AG

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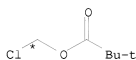
Q



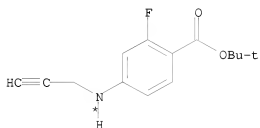
R



N

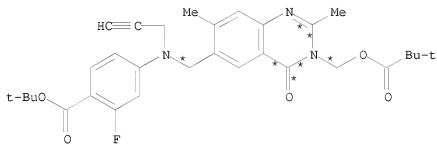


G



AI

6
STEPS
→



AG
YIELD 80%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et3N

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)
RCT R 75-36-5
CON SUBSTAGE(1) 2 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C
SUBSTAGE(3) 50 deg C -> 20 deg C

STAGE(3)
RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,
5-(bromomethyl)-1,2,3,4,7,7-hexachloro-
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 60 minutes
SUBSTAGE(3) 50 deg C -> 20 deg C

PRO M 838858-88-1
NTE regioselective

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)
SOL 68-12-2 DMF
CON SUBSTAGE(1) 6 hours, 90 deg C
SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)
RGT O 7440-66-6 Zn
CON SUBSTAGE(1) 60 deg C
SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0
NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0
RGT K 7647-01-0 HCl
PRO F 838858-86-9
SOL 67-63-0 Me2CHOH
CON SUBSTAGE(1) 60 minutes
SUBSTAGE(2) 30 deg C
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)
RGT H 584-08-7 K2CO3
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)
RCT G 18997-19-8
CON SUBSTAGE(1) 2.5 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)

RGT C 10035-10-6 HBr
 SOL 7732-18-5 Water, 64-19-7 AcOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)

RGT C 10035-10-6 HBr
 SOL 7732-18-5 Water, 64-19-7 AcOH
 CON SUBSTAGE(1) 2 hours, 60 deg C
 SUBSTAGE(2) 3 hours, 60 deg C
 SUBSTAGE(3) 60 deg C -> 16 deg C
 SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)

RGT AJ 144-55-8 NaHCO3
 SOL 7732-18-5 Water, 108-88-3 PhMe
 CON SUBSTAGE(1) 30 minutes, 65 deg C
 SUBSTAGE(2) 1 hour

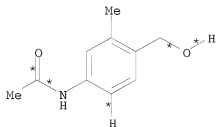
STAGE(2)

RCT AI 140373-03-1
 RGT AK 108-48-5 2,6-Lutidine
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) 105 deg C
 SUBSTAGE(2) 24 hours, 105 deg C
 SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(44) OF 45 COMPOSED OF RX(5), RX(4), RX(3), RX(2), RX(1)

RX(44) Q + R + N + G ==> B



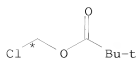
Q



R

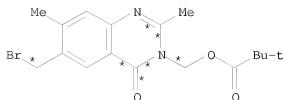


N



G

5
 STEPS
 →



● HBr

B
YIELD 89%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et3N
SOL 141-78-6 AcOEt
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RCT R 75-36-5
CON SUBSTAGE(1) 2 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C
SUBSTAGE(3) 50 deg C -> 20 deg C

STAGE(3)

RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,
5-(bromomethyl)-1,2,3,4,7,7-hexachloro-
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 60 minutes
SUBSTAGE(3) 50 deg C -> 20 deg C

PRO M 838858-88-1
NTE regioselective

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)

SOL 68-12-2 DMF
CON SUBSTAGE(1) 6 hours, 90 deg C
SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)

RGT O 7440-66-6 Zn
CON SUBSTAGE(1) 60 deg C
SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0
NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0

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RGT K 7647-01-0 HCl
 PRO F 838858-86-9
 SOL 67-63-0 Me2CHOH
 CON SUBSTAGE(1) 60 minutes
 SUBSTAGE(2) 30 deg C
 NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)
 RGT H 584-08-7 K2CO3
 SOL 67-68-5 DMSO
 CON SUBSTAGE(1) 50 deg C
 SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)
 RCT G 18997-19-8
 CON SUBSTAGE(1) 2.5 hours, 50 deg C
 SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

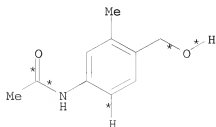
STAGE(1)
 RGT C 10035-10-6 HBr
 SOL 7732-18-5 Water, 64-19-7 AcOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)
 RGT C 10035-10-6 HBr
 SOL 7732-18-5 Water, 64-19-7 AcOH
 CON SUBSTAGE(1) 2 hours, 60 deg C
 SUBSTAGE(2) 3 hours, 60 deg C
 SUBSTAGE(3) 60 deg C -> 16 deg C
 SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(45) OF 45 COMPOSED OF RX(5), RX(4), RX(3), RX(2), RX(1), RX(9), RX(8),
 RX(7), RX(6)

RX(45) Q + R + N + G + AI + AC ==> X



Q

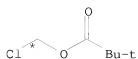


R

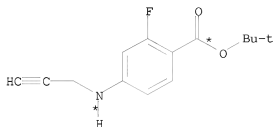


N

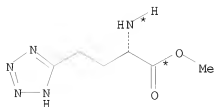
10/ 562,112



G

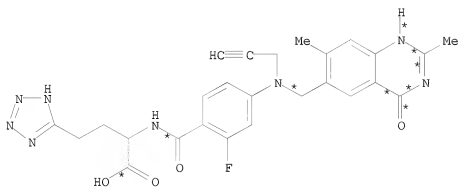


AI



AC

9
STEPS
→



X
YIELD 92%

RX(5) RCT Q 117523-91-8

STAGE(1)

RGT S 121-44-8 Et3N

SOL 141-78-6 AcOEt

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RCT R 75-36-5

CON SUBSTAGE(1) 2 hours, 50 deg C

SUBSTAGE(2) 30 minutes, 50 deg C
SUBSTAGE(3) 50 deg C -> 20 deg C

STAGE(3)
RGT T 1715-40-8 Bicyclo[2.2.1]hept-2-ene,
5-(bromomethyl)-1,2,3,4,7,7-hexachloro-
SOL 75-05-8 MeCN
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 60 minutes
SUBSTAGE(3) 50 deg C -> 20 deg C

PRO M 838858-88-1
NTE regioselective

RX(4) RCT M 838858-88-1, N 544-92-3

STAGE(1)
SOL 68-12-2 DMF
CON SUBSTAGE(1) 6 hours, 90 deg C
SUBSTAGE(2) 90 deg C -> 60 deg C

STAGE(2)
RGT O 7440-66-6 Zn
CON SUBSTAGE(1) 60 deg C
SUBSTAGE(2) 60 deg C -> 90 deg C

PRO J 838858-87-0
NTE inert, incremental addition of reagent in second stage

RX(3) RCT J 838858-87-0
RGT K 7647-01-0 HCl
PRO F 838858-86-9
SOL 67-63-0 Me2CHOH
CON SUBSTAGE(1) 60 minutes
SUBSTAGE(2) 30 deg C
NTE HCl gas used

RX(2) RCT F 838858-86-9

STAGE(1)
RGT H 584-08-7 K2CO3
SOL 67-68-5 DMSO
CON SUBSTAGE(1) 50 deg C
SUBSTAGE(2) 16 hours, 50 deg C

STAGE(2)
RCT G 18997-19-8
CON SUBSTAGE(1) 2.5 hours, 50 deg C
SUBSTAGE(2) 30 minutes, 50 deg C

PRO A 838858-85-8

RX(1) RCT A 838858-85-8

STAGE(1)
RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 60 deg C

STAGE(2)
RGT C 10035-10-6 HBr
SOL 7732-18-5 Water, 64-19-7 AcOH
CON SUBSTAGE(1) 2 hours, 60 deg C
SUBSTAGE(2) 3 hours, 60 deg C
SUBSTAGE(3) 60 deg C -> 16 deg C
SUBSTAGE(4) 18 hours, 16 deg C

PRO B 838858-84-7

RX(9) RCT B 838858-84-7

STAGE(1)
RGT AJ 144-55-8 NaHCO3
SOL 7732-18-5 Water, 108-88-3 PhMe
CON SUBSTAGE(1) 30 minutes, 65 deg C
SUBSTAGE(2) 1 hour

STAGE(2)
RCT AI 140373-03-1
RGT AK 108-48-5 2,6-Lutidine
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 105 deg C
SUBSTAGE(2) 24 hours, 105 deg C
SUBSTAGE(3) 105 deg C -> 65 deg C

PRO AG 153538-14-8

RX(8) RCT AG 153538-14-8

STAGE(1)
RGT AH 64-18-6 HCO2H
SOL 7732-18-5 Water
CON 5 hours, 40 deg C

STAGE(2)
RGT D 7732-18-5 Water
CON 3 hours

PRO AB 140373-09-7

RX(7) RCT AB 140373-09-7

STAGE(1)
RGT AD 7719-09-7 SOCl2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 30 minutes, 10 deg C
SUBSTAGE(2) 10 deg C -> 20 deg C

STAGE(2)
RCT AC 127105-49-1
RGT AE 7087-68-5 EtN(Pr-i)2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 3 hours, 10 deg C
SUBSTAGE(2) 16 hours

STAGE(3)
RGT E 64-19-7 AcOH

PRO W 247904-63-8

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NTE inert

RX(6) RCT W 247904-63-8

STAGE(1)

RGT Y 1310-73-2 NaOH
SOL 7732-18-5 Water, 109-99-9 THF
CON SUBSTAGE(1) 15 deg C
SUBSTAGE(2) 15 deg C -> 24 deg C
SUBSTAGE(3) 19 hours, 24 deg C

STAGE(2)

RGT Z 7631-90-5 NaHSO3
SOL 7732-18-5 Water
CON 40 minutes, 24 deg C

PRO X 153537-73-6

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 58 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:178643 CASREACT

TITLE: Synthesis and fastness properties of styryl and azo
disperse dyes derived from 6-nitro substituted
3-aryl-2-methyl-4(3H)-quinazolinone

AUTHOR(S): Bhatti, Harjinder Singh; Seshadri, Sambamurthy
CORPORATE SOURCE: Dyes Research Laboratory, University Institute of
Chemical Technology, University of Mumbai, Mumbai,
400019, India

SOURCE: Coloration Technology (2004), 120(4), 151-155
CODEN: CTOEAZ; ISSN: 1472-3581

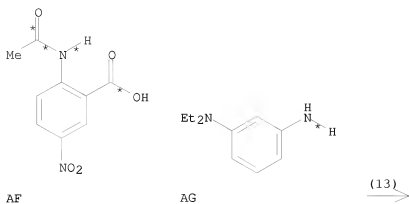
PUBLISHER: Society of Dyers and Colourists

DOCUMENT TYPE: Journal

LANGUAGE: English

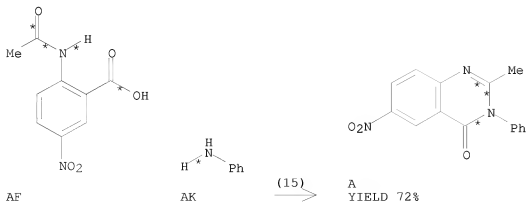
AB The synthesis of 6-nitro-substituted 3-aryl-2-methyl-4(3H)-quinazolinones
from readily available starting materials, such as isatoic anhydride, is
described. One of these, 3-phenyl-2-methyl-4(3H)-quinazolinone, has been
utilized to prepare a range of styryl disperse dyes for polyester. Novel
azo disperse dyes based on 6-nitro-3-[m-(diethylamino)phenyl]-2-methyl-
4(3H)-quinazolinone as coupling component are reported. The application
properties of the dyes on polyester and their fastness properties have
been evaluated, with the latter being disappointing.

RX(13) OF 57 ...AF + AG ==> Q...



RX(13) RCT AF 3558-18-7, AG 26513-20-2
 PRO Q 834881-82-2
 NTE no exptl. detail

RX(15) OF 57 ...AF + AK ==> A...



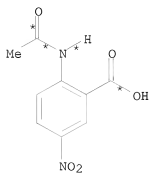
RX(15) RCT AF 3558-18-7, AK 62-53-3
 RGT AL 7719-12-2 PC13

10/ 562,112

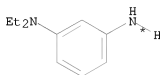
PRO A 966-91-6

RX(17) OF 57 COMPOSED OF RX(13), RX(7)

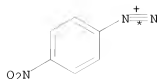
RX(17) AF + AG + R ==> S



AF

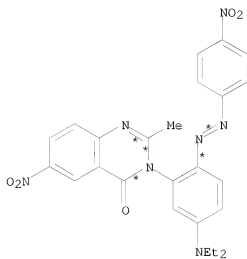


AG



R

2
STEPS
→



S
YIELD 75%

RX(13) RCT AF 3558-18-7, AG 26513-20-2
PRO Q 834881-82-2
NTE no exptl. detail

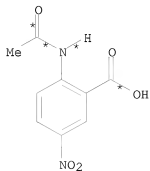
RX(7) RCT Q 834881-82-2, R 14368-49-1
RGT T 127-09-3 AcONa
PRO S 834881-76-4

10/ 562,112

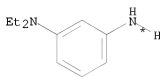
SOL 64-19-7 AcOH
 CON 2 - 3 hours, 0 - 5 deg C, pH 4 - 5
 NTE regioselective

RX(18) OF 57 COMPOSED OF RX(13), RX(8)

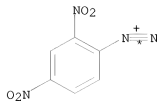
RX(18) AF + AG + V ==> W



AF

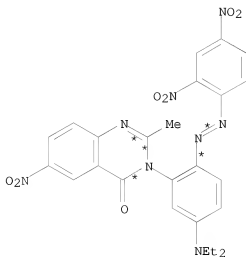


AG



V

2
 STEPS
 →

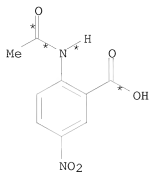


W
 YIELD 70%

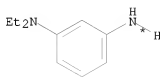
RX(13) RCT AF 3558-18-7, AG 26513-20-2
 PRO Q 834881-82-2
 NTE no exptl. detail

RX(8) RCT Q 834881-82-2, V 18300-85-1
 RGT T 127-09-3 AcONa
 PRO W 834881-77-5
 SOL 64-19-7 AcOH
 CON 2 - 3 hours, 0 - 5 deg C, pH 4 - 5
 NTE regioselective

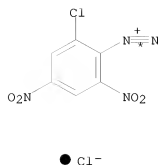
RX(19) OF 57 COMPOSED OF RX(13), RX(9)
 RX(19) AF + AG + X ==> Y



AF

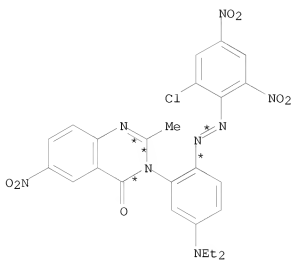


AG



X

2
 STEPS
 →



Y
 YIELD 65%

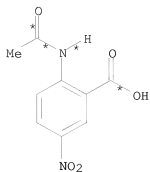
RX(13) RCT AF 3558-18-7, AG 26513-20-2
 PRO Q 834881-82-2
 NTE no exptl. detail

RX(9) RCT Q 834881-82-2, X 71668-09-2
 RGT T 127-09-3 AcONa
 PRO Y 834881-78-6
 SOL 64-19-7 AcOH
 CON 2 - 3 hours, 0 - 5 deg C, pH 4 - 5
 NTE regioselective

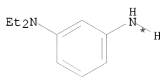
RX(20) OF 57 COMPOSED OF RX(13), RX(10)

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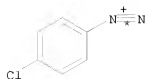
RX(20) AF + AG + Z ==> AA



AF

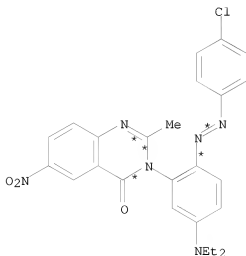


AG



Z

2
STEPS
→

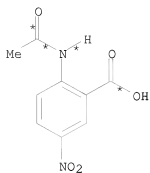


AA
YIELD 68%

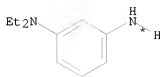
RX(13) RCT AF 3558-18-7, AG 26513-20-2
PRO Q 834881-82-2
NTE no exptl. detail

RX(10) RCT Q 834881-82-2, Z 17333-85-6
RGT T 127-09-3 AcONa
PRO AA 834881-79-7
SOL 64-19-7 AcOH
CON 2 - 3 hours, 0 - 5 deg C, pH 4 - 5
NTE regioselective

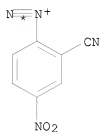
RX(21) OF 57 COMPOSED OF RX(13), RX(11)
RX(21) AF + AG + AB ==> AC



AF

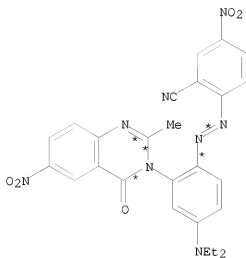


AG



AB

2
STEPS
→

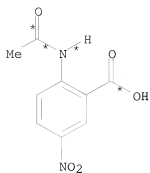


AC
YIELD 76%

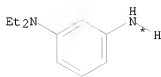
RX(13) RCT AF 3558-18-7, AG 26513-20-2
PRO Q 834881-82-2
NTE no exptl. detail

RX(11) RCT Q 834881-82-2, AB 66751-54-0
RGT T 127-09-3 AcONa
PRO AC 834881-80-0
SOL 64-19-7 AcOH
CON 2 - 3 hours, 0 - 5 deg C, pH 4 - 5
NTE regioselective

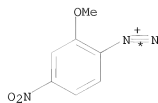
RX(22) OF 57 COMPOSED OF RX(13), RX(12)
RX(22) AF + AG + AD ==> AE



AF

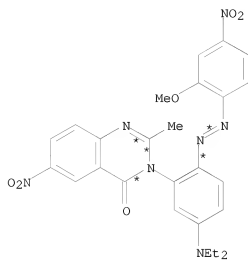


AG



AD

2
STEPS
→



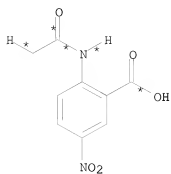
AE
YIELD 75%

RX(13) RCT AF 3558-18-7, AG 26513-20-2
PRO Q 834881-82-2
NTE no exptl. detail

RX(12) RCT Q 834881-82-2, AD 27761-26-8
RGT T 127-09-3 AcONa
PRO AE 834881-81-1
SOL 64-19-7 AcOH
CON 2 - 3 hours, 0 - 5 deg C, pH 4 - 5
NTE regioselective

RX(24) OF 57 COMPOSED OF RX(15), RX(1)

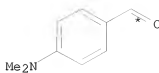
RX(24) AF + AK + B ==> C



AF

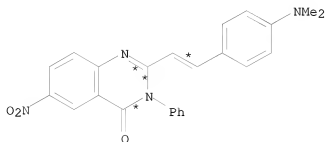


AK



B

2
STEPS
→



C

YIELD 76%

RX(15) RCT AF 3558-18-7, AK 62-53-3
RGT AL 7719-12-2 PC13
PRO A 966-91-6

RX(1) RCT A 966-91-6, B 100-10-7

STAGE(1)

RGT D 10025-87-3 POC13

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 3 hours, reflux

SUBSTAGE(3) cooled

STAGE(2)

RGT E 497-19-8 Na2CO3

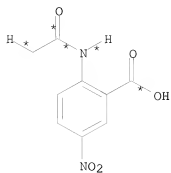
SOL 7732-18-5 Water

CON pH 5

PRO C 834881-70-8

RX(25) OF 57 COMPOSED OF RX(15), RX(2)

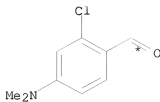
RX(25) AF + AK + G ==> H



AF

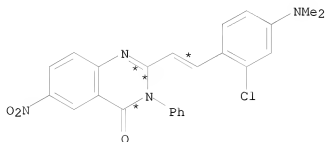


AK



G

2
STEPS
→



H
YIELD 70%

RX(15) RCT AF 3558-18-7, AK 62-53-3
RGT AL 7719-12-2 PC13
PRO A 966-91-6

RX(2) RCT A 966-91-6, G 1424-66-4

STAGE(1)

RGT D 10025-87-3 POC13

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 3 hours, reflux

SUBSTAGE(3) cooled

STAGE(2)

RGT E 497-19-8 Na2CO3

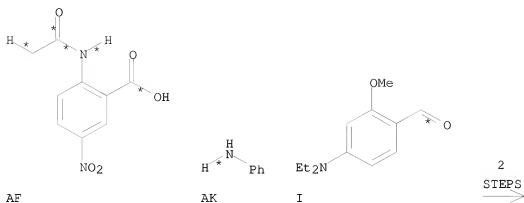
SOL 7732-18-5 Water

CON pH 5

PRO H 834881-71-9

RX(26) OF 57 COMPOSED OF RX(15), RX(3)

RX(26) AF + AK + I ==> J



J
YIELD 72%

RX(15) RCT AF 3558-18-7, AK 62-53-3
 RGT AL 7719-12-2 PC13
 PRO A 966-91-6

RX(3) RCT A 966-91-6, I 55586-68-0

STAGE(1)

RGT D 10025-87-3 POC13
CON SUBSTAGE(1) room temperature -> reflux
 SUBSTAGE(2) 3 hours, reflux
 SUBSTAGE(3) cooled

STAGE(2)

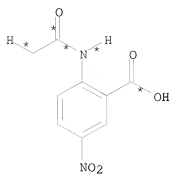
RGT E 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON pH 5

PRO J 834881-72-0

RX(27) OF 57 COMPOSED OF RX(15), RX(4)

RX(27) AF + AK + K ==> L

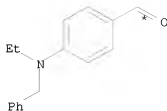
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AF

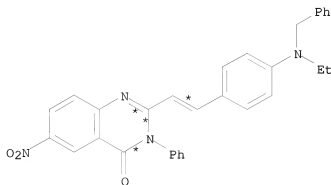


AK



K

2
STEPS
→



L

YIELD 67%

RX(15) RCT AF 3558-18-7, AK 62-53-3
RGT AL 7719-12-2 PC13
PRO A 966-91-6

RX(4) RCT A 966-91-6, K 67676-47-5

STAGE(1)

RGT D 10025-87-3 POC13

CON SUBSTAGE(1) room temperature -> reflux

SUBSTAGE(2) 3 hours, reflux

SUBSTAGE(3) cooled

STAGE(2)

RGT E 497-19-8 Na2CO3

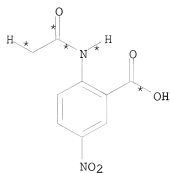
SOL 7732-18-5 Water

CON pH 5

PRO L 834881-73-1

RX(28) OF 57 COMPOSED OF RX(15), RX(5)

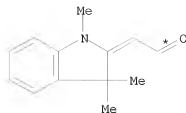
RX(28) AF + AK + M ==> N



AF

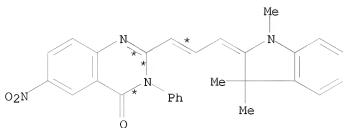


AK



M

2
STEPS
→



N
YIELD 73%

RX(15) RCT AF 3558-18-7, AK 62-53-3
RGT AL 7719-12-2 PCl3
PRO A 966-91-6

RX(5) RCT A 966-91-6, M 84-83-3

STAGE(1)

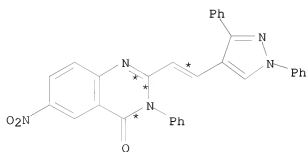
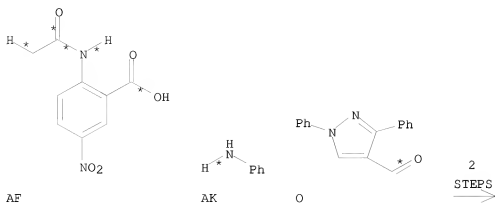
RGT D 10025-87-3 POC13
CON SUBSTAGE(1) room temperature -> reflux
SUBSTAGE(2) 3 hours, reflux
SUBSTAGE(3) cooled

STAGE(2)

RGT E 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON pH 5

PRO N 834881-74-2

RX(29) OF 57 COMPOSED OF RX(15), RX(6)
RX(29) AF + AK + O ==> P



P
YIELD 75%

RX(15) RCT AF 3558-18-7, AK 62-53-3
 RGT AL 7719-12-2 PCl3
 PRO A 966-91-6

RX(6) RCT A 966-91-6, O 21487-45-6

STAGE(1)

RGT D 10025-87-3 POC13
CON SUBSTAGE(1) room temperature -> reflux
 SUBSTAGE(2) 3 hours, reflux
 SUBSTAGE(3) cooled

STAGE(2)

RGT E 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON pH 5

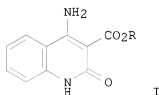
PRO P 834881-75-3

REFERENCE COUNT:

39

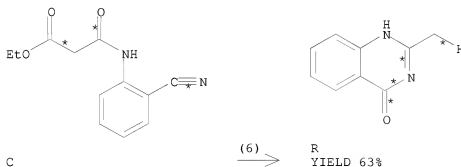
THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 59 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 142:176655 CASREACT
 TITLE: Synthesis and structure of
 1H-4-amino-2-oxoquinoline-3-carboxylic acid esters
 AUTHOR(S): Ukrainets, I. V.; Bezuglyi, P. A.; Nikola, Skaif;
 Gorokhova, O. V.; Sidorenko, L. V.
 CORPORATE SOURCE: Nats. Farm. Univ., Kharkov, 61002, Ukraine
 SOURCE: Zhurnal Organichnoi ta Farmatsevtichnoi Khimii (2004),
 2(1), 39-44
 CODEN: ZOFKAM
 PUBLISHER: Natsional'nii Farmatsevtichnii Universitet
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



AB Two approaches to the synthesis of 1H-4-amino-2-oxoquinoline-3-carboxylic acid esters I (R = Me, Et) are discussed. NMR spectroscopy studies and X-ray diffraction anal. established that these esters exist in DMSO-d6 solution and in the solid state exclusively as 4-amino-2-oxo tautomers shown.

RX(6) OF 18 ...C ==> R



RX(6) RCT C 130427-06-4

STAGE(1)

RGT Q 1310-58-3 KOH
 SOL 7732-18-5 Water
 CON 5 hours, reflux

STAGE(2)

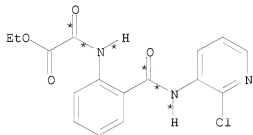
RGT H 7647-01-0 HCl

SOL 7732-18-5 Water
 CON room temperature, pH 4

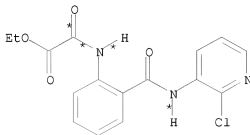
PRO R 1769-24-0

L3 ANSWER 60 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 142:155910 CASREACT
 TITLE: Intramolecular nucleophilic aromatic substitution
 reaction of 2-carboxamido-3-arylquinazolin-4-ones and
 its application to the synthesis of secondary aryl
 amines
 AUTHOR(S): Fuwa, Haruhiko; Kobayashi, Toshitake; Tokitoh,
 Takashi; Torii, Yukiko; Natsugari, Hideaki
 CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, University
 of Tokyo, Tokyo, 113-0033, Japan
 SOURCE: Synlett (2004), (14), 2497-2500
 CODEN: SYNLES; ISSN: 0936-5214
 PUBLISHER: Georg Thieme Verlag
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A novel intramol. nucleophilic aromatic substitution reaction of
 2-carboxamido-3-arylquinazolin-4-one derivs. induced by base treatment and
 its application to the expeditious synthesis of secondary aryl amines,
 including diaryl amines, are described.

RX(2) OF 83 ...2 C ==> F + G...

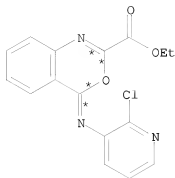


C

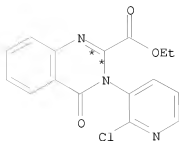


C

(2) →



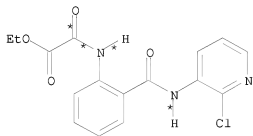
F



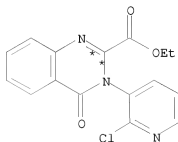
G

RX(2) RCT C 830324-66-8
 RGT H 7087-68-5 EtN(Pr-i)2, I 7553-56-2 I2, J 603-35-0 PPh3
 PRO F 830324-67-9, G 830324-68-0
 SOL 75-09-2 CH2Cl2
 CON 0 deg C -> room temperature
 NTE Snider reaction

RX(3) OF 83 ...C ==> G...



C



G
 YIELD 91%

RX(3) RCT C 830324-66-8

STAGE(1)

RGT H 7087-68-5 EtN(Pr-i)2, I 7553-56-2 I2, J 603-35-0 PPh3
 SOL 75-09-2 CH2Cl2
 CON 0 deg C -> room temperature

STAGE(2)

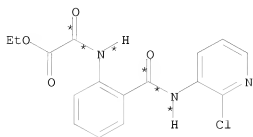
RGT L 123-75-1 Pyrrolidine
 SOL 109-99-9 THF, 64-19-7 AcOH
 CON reflux

PRO G 830324-68-0
 NTE chemoselective

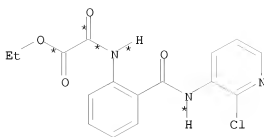
10/ 562,112

RX(37) OF 83 COMPOSED OF RX(2), RX(4)

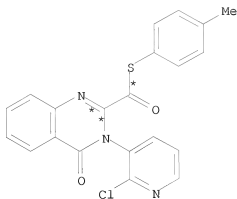
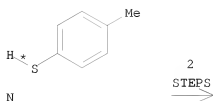
RX(37) 2 C + N ==> O



C



C



O

YIELD 87%

RX(2) RCT C 830324-66-8
 RGT H 7087-68-5 EtN(Pr-i)2, I 7553-56-2 I2, J 603-35-0 PPh3
 PRO F 830324-67-9, G 830324-68-0
 SOL 75-09-2 CH2Cl2
 CON 0 deg C -> room temperature
 NTE Snider reaction

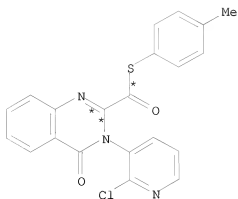
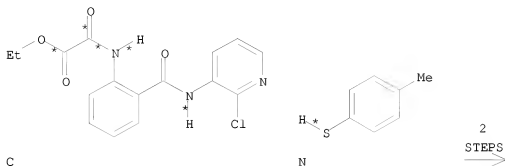
RX(4) RCT G 830324-68-0, N 106-45-6
 RGT P 75-24-1 AlMe3
 PRO O 830324-69-1
 SOL 75-09-2 CH2Cl2

10/ 562,112

CON 0 deg C -> room temperature

RX(43) OF 83 COMPOSED OF RX(3), RX(4)

RX(43) C + N ==> O



YIELD 87%

RX(3) RCT C 830324-66-8

STAGE(1)

RGT H 7087-68-5 EtN(Pr-i)₂, I 7553-56-2 I₂, J 603-35-0 PPh₃

SOL 75-09-2 CH₂Cl₂

CON 0 deg C -> room temperature

STAGE(2)

RGT L 123-75-1 Pyrrolidine

SOL 109-99-9 THF, 64-19-7 AcOH

CON reflux

PRO G 830324-68-0

NTE chemoselective

RX(4) RCT G 830324-68-0, N 106-45-6

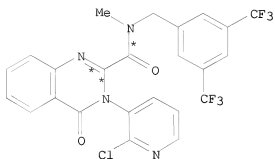
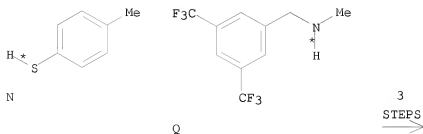
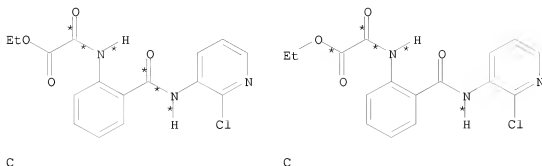
RGT P 75-24-1 AlMe₃

PRO O 830324-69-1

10/ 562,112

SOL 75-09-2 CH2Cl2
CON 0 deg C -> room temperature

RX(68) OF 83 COMPOSED OF RX(2), RX(4), RX(5)
RX(68) 2 C + N + Q ==> R



R
YIELD 100%

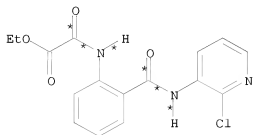
RX(2) RCT C 830324-66-8
RGT H 7087-68-5 EtN(Pr-i)2, I 7553-56-2 I2, J 603-35-0 PPh3
PRO F 830324-67-9, G 830324-68-0
SOL 75-09-2 CH2Cl2
CON 0 deg C -> room temperature
NTE Snider reaction

10/ 562,112

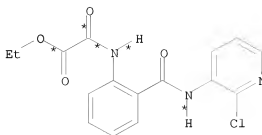
RX(4) RCT G 830324-68-0, N 106-45-6
 RGT P 75-24-1 AlMe3
 PRO O 830324-69-1
 SOL 75-09-2 CH2Cl2
 CON 0 deg C -> room temperature

RX(5) RCT O 830324-69-1, Q 159820-24-3
 RGT S 2966-50-9 F3CCO2 Ag
 PRO R 830324-71-5
 SOL 109-99-9 THF, 108-88-3 PhMe
 CON 60 deg C

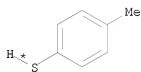
RX(69) OF 83 COMPOSED OF RX(2), RX(4), RX(6)
 RX(69) 2 C + N + U ==> V



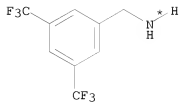
C



C



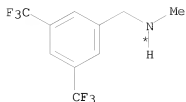
N



U

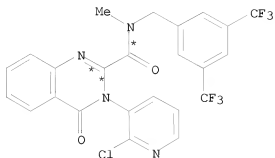
3
 STEPS
 →

10/ 562,112



Q

3
STEPS
→



R
YIELD 100%

RX(3) RCT C 830324-66-8

STAGE(1)

RGT H 7087-68-5 EtN(Pr-i)2, I 7553-56-2 I2, J 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON 0 deg C -> room temperature

STAGE(2)

RGT L 123-75-1 Pyrrolidine
SOL 109-99-9 THF, 64-19-7 AcOH
CON reflux

PRO G 830324-68-0
NTE chemoselective

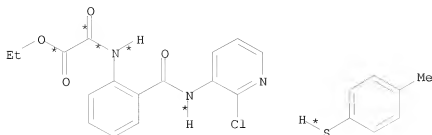
RX(4) RCT G 830324-68-0, N 106-45-6
RGT P 75-24-1 AlMe3
PRO O 830324-69-1
SOL 75-09-2 CH2Cl2
CON 0 deg C -> room temperature

RX(5) RCT O 830324-69-1, Q 159820-24-3
RGT S 2966-50-9 F3CCO2 Ag
PRO R 830324-71-5
SOL 109-99-9 THF, 108-88-3 PhMe
CON 60 deg C

RX(71) OF 83 COMPOSED OF RX(3), RX(4), RX(6)

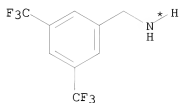
10/ 562,112

RX(71) C + N + U ==> V



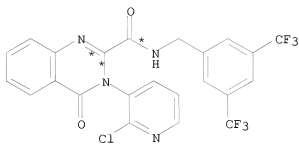
C

N



U

3
STEPS
→



V

YIELD 100%

RX(3) RCT C 830324-66-8

STAGE(1)

RGT H 7087-68-5 EtN(Pr-i)₂, I 7553-56-2 I₂, J 603-35-0 PPh₃
 SOL 75-09-2 CH₂Cl₂
 CON 0 deg C -> room temperature

STAGE(2)

RGT L 123-75-1 Pyrrolidine
 SOL 109-99-9 THF, 64-19-7 AcOH
 CON reflux

PRO G 830324-68-0

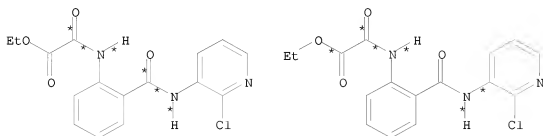
10/ 562,112

NTE chemoselective

RX(4) RCT G 830324-68-0, N 106-45-6
 RGT P 75-24-1 AlMe3
 PRO O 830324-69-1
 SOL 75-09-2 CH2Cl2
 CON 0 deg C -> room temperature

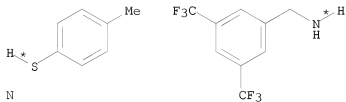
RX(6) RCT O 830324-69-1, U 85068-29-7
 RGT S 2966-50-9 F3CCO2 Ag
 PRO V 830324-70-4
 SOL 109-99-9 THF, 108-88-3 PhMe
 CON 60 deg C

RX(77) OF 83 COMPOSED OF RX(2), RX(4), RX(6), RX(7)
 RX(77) 2 C + N + U + W ==> X



C

C



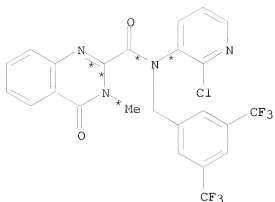
N

U

H₃C-I

W

4
 STEPS
 ➔



X

YIELD 81%

RX(2) RCT C 830324-66-8
 RGT H 7087-68-5 EtN(Pr-i)2, I 7553-56-2 I2, J 603-35-0 PPh3
 PRO F 830324-67-9, G 830324-68-0
 SOL 75-09-2 CH2Cl2
 CON 0 deg C -> room temperature
 NTE Snider reaction

RX(4) RCT G 830324-68-0, N 106-45-6
 RGT P 75-24-1 AlMe3
 PRO O 830324-69-1
 SOL 75-09-2 CH2Cl2
 CON 0 deg C -> room temperature

RX(6) RCT O 830324-69-1, U 85068-29-7
 RGT S 2966-50-9 F3CCO2 Ag
 PRO V 830324-70-4
 SOL 109-99-9 THF, 108-88-3 PhMe
 CON 60 deg C

RX(7) RCT V 830324-70-4

STAGE(1)

RGT Y 7646-69-7 NaH
 SOL 68-12-2 DMF
 CON 1 hour, 0 deg C -> room temperature

STAGE(2)

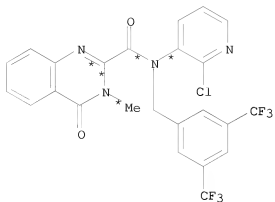
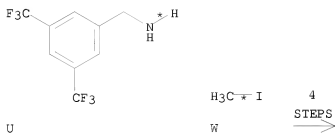
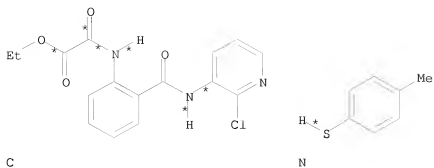
RCT W 74-88-4
 CON 1 hour, 0 deg C -> room temperature

PRO X 830324-72-6
 NTE regioselective

RX(78) OF 83 COMPOSED OF RX(3), RX(4), RX(6), RX(7)

RX(78) C + N + U + W ==> X

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YIELD 81%

RX(3) RCT C 830324-66-8

STAGE(1)

RGT H 7087-68-5 EtN(Pr-i)2, I 7553-56-2 12, J 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON 0 deg C -> room temperature

STAGE(2)

RGT L 123-75-1 Pyrrolidine

SOL 109-99-9 THF, 64-19-7 AcOH

CON reflux

PRO G 830324-68-0
NTE chemoselectiveRX(4) RCT G 830324-68-0, N 106-45-6
RGT P 75-24-1 AlMe3
PRO O 830324-69-1
SOL 75-09-2 CH2Cl2
CON 0 deg C -> room temperatureRX(6) RCT O 830324-69-1, U 85068-29-7
RGT S 2966-50-9 F3CCO2 Ag
PRO V 830324-70-4
SOL 109-99-9 THF, 108-88-3 PhMe
CON 60 deg C

RX(7) RCT V 830324-70-4

STAGE(1)

RGT Y 7646-69-7 NaH
SOL 68-12-2 DMF
CON 1 hour, 0 deg C -> room temperature

STAGE(2)

RCT W 74-88-4
CON 1 hour, 0 deg C -> room temperaturePRO X 830324-72-6
NTE regioselectiveREFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 61 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:114314 CASREACT

TITLE: Intramolecular Hetero Diels-Alder (Povarov) Approach
to the Synthesis of the Alkaloids Luotonin A and
Camptothecin

AUTHOR(S): Twin, Heather; Batey, Robert A.

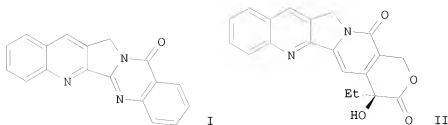
CORPORATE SOURCE: Department of Chemistry, University of Toronto,
Toronto, ON, M5S 3H6, Can.SOURCE: Organic Letters (2004), 6(26), 4913-4916
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

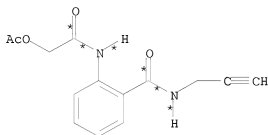
GI



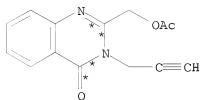
AB Pyrrolo[3,4-b]quinolines can be formed through the coupling of anilines with N-propargylic substituted heterocyclic aldehydes in the presence of mild Lewis acid catalysts. The coupling proceeds through sequential imine formation and a formal intramol. aza-Diels-Alder (Povarov) reaction. This approach was applied in a total synthesis of luotonin A (I) and a formal synthesis of camptothecin (II).

RX(19) OF 47 COMPOSED OF RX(7), RX(8)

RX(19) U ==> AD



2
STEPS
→



YIELD 85%

RX(7) RCT U 823235-08-1

STAGE(1)

RGT Y 7087-68-5 EtN(Pr-i)₂, Z 7553-56-2 I₂, AA 603-35-0 PPh₃

SOL 75-09-2 CH₂Cl₂

CON 5 hours, room temperature

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STAGE(2)

RGT AB 497-19-8 Na2CO3

SOL 7732-18-5 Water

PRO X 823235-09-2

RX(8) RCT X 823235-09-2

STAGE(1)

RGT AE 110-89-4 Piperidine

SOL 141-78-6 AcOEt

CON 1 hour, room temperature

STAGE(2)

RGT AF 7631-86-9 SiO2

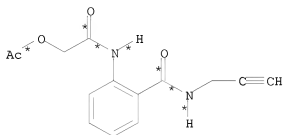
SOL 141-78-6 AcOEt

CON overnight, room temperature

PRO AD 823235-10-5

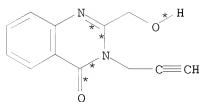
RX(33) OF 47 COMPOSED OF RX(7), RX(8), RX(13)

RX(33) U ==> AH



U

3
STEPS
→



AH

YIELD 83%

RX(7) RCT U 823235-08-1

STAGE(1)

RGT Y 7087-68-5 EtN(Pr-i)2, Z 7553-56-2 I2, AA 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON 5 hours, room temperature

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STAGE(2)

RGT AB 497-19-8 Na2CO3

SOL 7732-18-5 Water

PRO X 823235-09-2

RX(8) RCT X 823235-09-2

STAGE(1)

RGT AE 110-89-4 Piperidine

SOL 141-78-6 AcOEt

CON 1 hour, room temperature

STAGE(2)

RGT AF 7631-86-9 SiO2

SOL 141-78-6 AcOEt

CON overnight, room temperature

PRO AD 823235-10-5

RX(13) RCT AD 823235-10-5

STAGE(1)

RGT AT 1310-73-2 NaOH

SOL 7732-18-5 Water, 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RGT O 7647-01-0 HCl

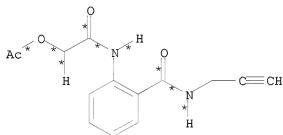
SOL 7732-18-5 Water

CON pH 4.5

PRO AH 823235-13-8

RX(36) OF 47 COMPOSED OF RX(7), RX(8), RX(13), RX(9)

RX(36) U ==> A

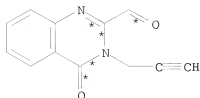


4

STEPS

U





A

YIELD 78%

RX(7) RCT U 823235-08-1

STAGE(1)

RGT Y 7087-68-5 EtN(Pr-i)2, Z 7553-56-2 I2, AA 603-35-0 PPh3

SOL 75-09-2 CH2Cl2

CON 5 hours, room temperature

STAGE(2)

RGT AB 497-19-8 Na2CO3

SOL 7732-18-5 Water

PRO X 823235-09-2

RX(8) RCT X 823235-09-2

STAGE(1)

RGT AE 110-89-4 Piperidine

SOL 141-78-6 AcOEt

CON 1 hour, room temperature

STAGE(2)

RGT AF 7631-86-9 SiO2

SOL 141-78-6 AcOEt

CON overnight, room temperature

PRO AD 823235-10-5

RX(13) RCT AD 823235-10-5

STAGE(1)

RGT AT 1310-73-2 NaOH

SOL 7732-18-5 Water, 109-99-9 THF

CON 1 hour, room temperature

STAGE(2)

RGT O 7647-01-0 HCl

SOL 7732-18-5 Water

CON pH 4.5

PRO AH 823235-13-8

RX(9) RCT AH 823235-13-8

RGT AI 110-86-1 Pyridine, AJ 87413-09-0 Martin's reagent

PRO A 823235-11-6

SOL 75-09-2 CH2Cl2

CON SUBSTAGE(1) 15 minutes, 0 deg C

SUBSTAGE(2) 1 hour, room temperature
 SUBSTAGE(3) 4 hours, room temperature

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 62 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:93763 CASREACT

TITLE: Improved synthesis of
 3,4-dihydro-2,6-dimethyl-4-oxoquinazoline

AUTHOR(S): Chen, Shiyao; Lin, Jimao; Qin, Bingjie

CORPORATE SOURCE: School of Chemistry and Chemical Engineering, Shandong
 University, Jinan, 250100, Peop. Rep. China

SOURCE: Organic Preparations and Procedures International
 (2004), 36(3), 277-279

CODEN: OPPIAK; ISSN: 0030-4948

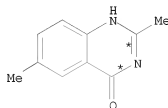
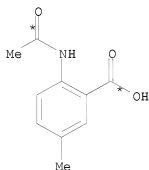
PUBLISHER: Organic Preparations and Procedures, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The preparation of title compound is described. Thus, potassium permanganate oxidation of 2,4-dimethylacetanilide gave 23% 2-acetamido-5-methylbenzoic acid which on cyclization with NH₄OAc/Ac₂O gave title compound

RX(2) OF 3 ...B ==> G



B $\xrightarrow{(2)}$ G
 YIELD 20%

RX(2) RCT B 67081-68-9

STAGE(1)

SOL 108-24-7 Ac₂O

CON 3 hours, reflux

STAGE(2)

RGT H 631-61-8 NH₄OAc

CON 16 hours, reflux

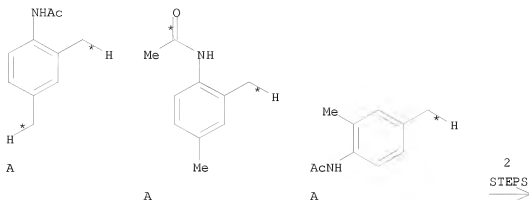
PRO G 18731-19-6

NTE petroleum ether solvent at 1st step

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RX(3) OF 3 COMPOSED OF RX(1), RX(2)

RX(3) 3 A ==> G



G
YIELD 20%

RX(1) RCT A 2050-43-3
RGT E 7722-64-7 KMnO4
PRO B 67081-68-9, C 37901-92-1, D 7501-68-0
SOL 7732-18-5 Water
CON 80 deg C

RX(2) RCT B 67081-68-9

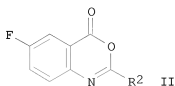
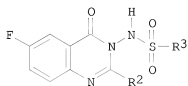
STAGE(1)
SOL 108-24-7 Ac2O
CON 3 hours, reflux

STAGE(2)
RGT H 631-61-8 NH4OAc
CON 16 hours, reflux

PRO G 18731-19-6
NTE petroleum ether solvent at 1st step

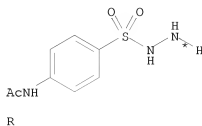
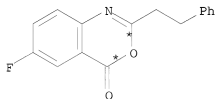
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 63 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 142:23247 CASREACT
 TITLE: Novel parallel synthesis of
 N-(4-oxo-2-substituted-4H-quinazolin-3-yl)-substituted
 sulfonamides
 AUTHOR(S): Zhou, Yufen; Murphy, Douglas E.; Sun, Zhongxiang;
 Gregor, Vlad E.
 CORPORATE SOURCE: Department of Medicinal Chemistry, Anadys
 Pharmaceuticals Inc., San Diego, CA, 92121, USA
 SOURCE: Tetrahedron Letters (2004), 45(43), 8049-8051
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



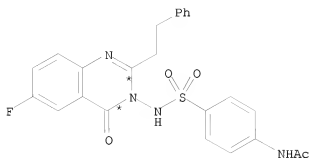
AB A general method was developed to synthesize a class of
 N-(4-oxo-2-substituted-4H-quinazolin-3-yl)-substituted sulfonamides I (R2
 = PhCH2, PhCH2CH2, 2-thiophenemethylene, R3 = 4-HO2CC6H4, 2-ClC6H4,
 4-Me3CC6H4, etc.) in moderate to good yield by reacting benzoxazines II
 with R3SO2NHNH2 by melting the compds. together at 130°C for 30
 min. This new method can be applied in both single compound and parallel
 synthesis. About 90 compds. with a variety of substituents were
 synthesized using this method in a parallel fashion.

RX(9) OF 182 ...C + R ==> S



(9) →

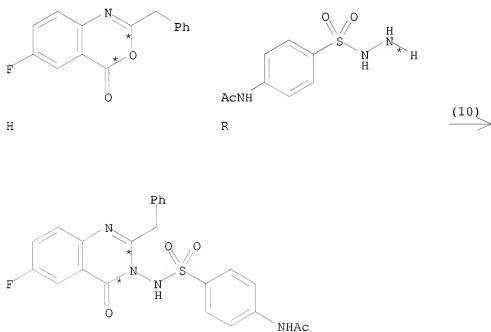
10/ 562,112



S
YIELD 99%

RX(9) RCT C 799797-25-4, R 3989-50-2
 PRO S 799797-38-9
 CON 30 minutes, 130 deg C
 NTE safety - potential uncontrollable decomposition, safety shield
 recommended, scale .2 mmol or smaller recommended;
 combinatorial, parallel synthesis; no solvent

RX(10) OF 182 ...H + R ==> T



T
YIELD 94%

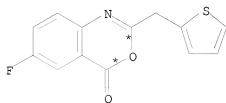
RX(10) RCT H 799797-27-6, R 3989-50-2
 PRO T 799797-39-0

10/ 562,112

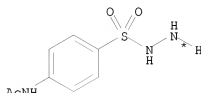
CON 30 minutes, 130 deg C

NTE safety - potential uncontrollable decomposition, safety shield
recommended, scale .2 mmol or smaller recommended;
combinatorial, parallel synthesis; no solvent

RX(12) OF 182 ...L + R ==> V

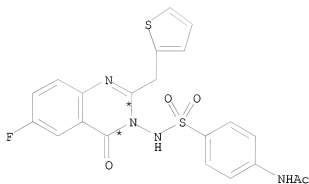


L



R

(12)



V

YIELD 99%

RX(12) RCT L 799797-28-7, R 3989-50-2

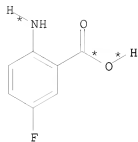
PRO V 799797-41-4

CON 30 minutes, 130 deg C

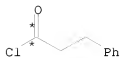
NTE safety - potential uncontrollable decomposition, safety shield
recommended, scale .2 mmol or smaller recommended;
combinatorial, parallel synthesis; no solvent

RX(95) OF 182 COMPOSED OF RX(1), RX(9)

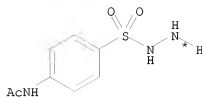
RX(95) A + B + R ==> S



A

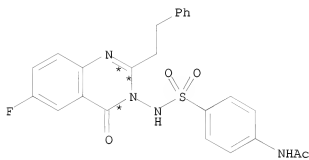


B



R

2
STEPS
→



S
YIELD 99%

RX(1) RCT A 446-08-2, B 645-45-4

STAGE(1)

RGT D 121-44-8 Et3N
SOL 75-09-2 CH2Cl2
CON room temperature

STAGE(2)

RGT E 108-24-7 Ac2O
CON 1 hour, 165 deg C

PRO C 799797-25-4

RX(9) RCT C 799797-25-4, R 3989-50-2

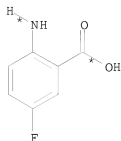
PRO S 799797-38-9

CON 30 minutes, 130 deg C

NTE safety - potential uncontrollable decomposition, safety shield
recommended, scale .2 mmol or smaller recommended;
combinatorial, parallel synthesis; no solvent

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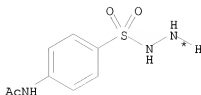
RX(117) OF 182 COMPOSED OF RX(2), RX(10)
RX(117) A + G + R ==> T



A

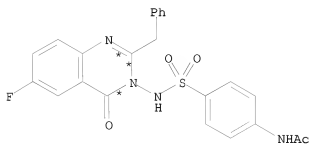


G



R

2
STEPS
→



T
YIELD 94%

RX(2) RCT A 446-08-2, G 103-80-0

STAGE(1)

RGT D 121-44-8 Et3N
SOL 75-09-2 CH2Cl2
CON room temperature

STAGE(2)

RGT E 108-24-7 Ac2O
CON 1 hour, 165 deg C

PRO H 799797-27-6

RX(10) RCT H 799797-27-6, R 3989-50-2

PRO T 799797-39-0

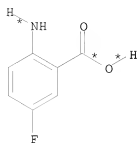
CON 30 minutes, 130 deg C

NTE safety - potential uncontrollable decomposition, safety shield recommended, scale .2 mmol or smaller recommended;
combinatorial, parallel synthesis; no solvent

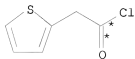
10/ 562,112

RX(160) OF 182 COMPOSED OF RX(4), RX(12)

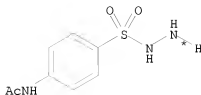
RX(160) A + K + R ==> V



A

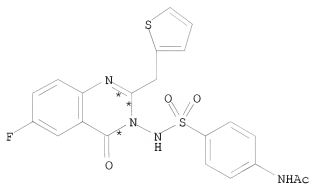


K



R

2
STEPS
=>



V

YIELD 99%

RX(4) RCT A 446-08-2, K 39098-97-0

STAGE(1)

RGT D 121-44-8 Et3N

SOL 75-09-2 CH2Cl2

CON room temperature

STAGE(2)

RGT E 108-24-7 Ac2O

CON 1 hour, 165 deg C

PRO L 799797-28-7

RX(12) RCT L 799797-28-7, R 3989-50-2

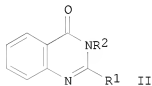
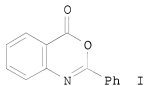
PRO V 799797-41-4

CON 30 minutes, 130 deg C

NTE safety - potential uncontrollable decomposition, safety shield recommended, scale .2 mmol or smaller recommended; combinatorial, parallel synthesis; no solvent

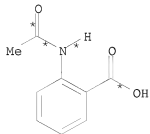
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 64 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 142:23246 CASREACT
 TITLE: Microwave irradiated one flask synthesis of 2,3-disubstituted quinazolin-4-ones
 AUTHOR(S): Tripathy, Pradeep K.
 CORPORATE SOURCE: Department of Chemistry, North Eastern Regional Institute of Science and Technology, Itanagar, 791 109, India
 SOURCE: Journal of the Institution of Chemists (India) (2003), 75(6), 179-180
 CODEN: JOICA7; ISSN: 0020-3254
 PUBLISHER: Institution of Chemists (India)
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

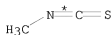


AB Microwave-induced reaction of N-acetyl- and N-benzoylanthranilic acid with Me and Ph isothiocyanate gave benzoxazinone I and quinazolinones II (R1 = R2 = Me, Ph; R1 = Me, R2 = Ph).

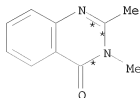
RX(1) OF 4 A + B ==> C



A



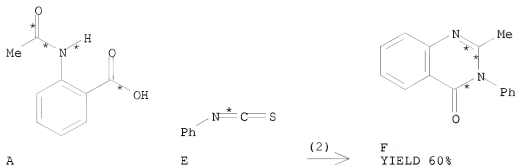
B



C
YIELD 35%

RX(1) RCT A 89-52-1, B 556-61-6
 PRO C 1769-25-1
 CAT 110-86-1 Pyridine
 CON 5 minutes
 NTE microwave irradiation, no solvent

RX(2) OF 4 A + E ==> F

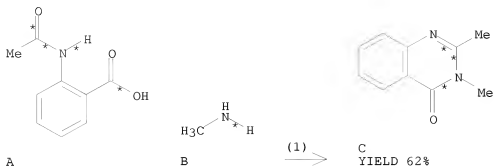


RX(2) RCT A 89-52-1, E 103-72-0
 PRO F 2385-23-1
 CAT 110-86-1 Pyridine
 CON 5 minutes
 NTE microwave irradiation, no solvent

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 65 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 141:366195 CASREACT
 TITLE: Benzenesulfonyl chloride as a cyclocondensing agent in one pot synthesis of 3-substituted 2-methylquinazolin-4-ones
 AUTHOR(S): Tripathy, Pradeep K.
 CORPORATE SOURCE: Department of Chemistry, North Eastern Regional Institute of Science & Technology, Itanagar, 791 109, India
 SOURCE: Journal of the Institution of Chemists (India) (2004), 76(1), 6-8
 CODEN: JOICA7; ISSN: 0020-3254
 PUBLISHER: Institution of Chemists (India)
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The objective of the present study was to develop a method for the rapid and facile synthesis of 3-substituted 2-methyl-quinazolin-4-ones by using benzenesulfonyl chloride as cyclocondensing agent. Benzenesulfonyl chloride is easily available as an effective cyclocondensing agent for N-acetyl-L-tryptophan. Considering the easy availability of the starting materials, speed of the reaction, the mild exptl. conditions and the simplicity of the workup, the present method appears to be useful.

RX(1) OF 3 A + B ==> C



RX(1) RCT A 89-52-1

STAGE(1)

RGT D 98-09-9 PhSO₂Cl, E 121-44-8 Et₃N

SOL 71-43-2 Benzene

CON room temperature

STAGE(2)

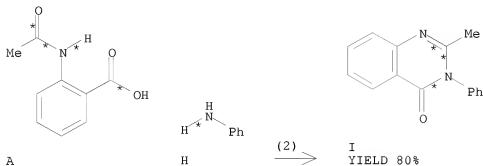
RCT B 74-89-5

SOL 64-19-7 AcOH

CON 4 hours, reflux

PRO C 1769-25-1

RX(2) OF 3 A + H ==> I



RX(2) RCT A 89-52-1

STAGE(1)

RGT D 98-09-9 PhSO₂Cl, E 121-44-8 Et₃N

SOL 71-43-2 Benzene

CON room temperature

STAGE(2)

RCT H 62-53-3

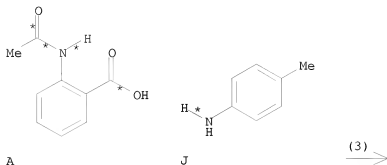
SOL 64-19-7 AcOH

CON 4 hours, reflux

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PRO I 2385-23-1

RX(3) OF 3 A + J ==> K



K
YIELD 78%

RX(3) RCT A 89-52-1

STAGE(1)

RGT D 98-09-9 PhSO₂Cl, E 121-44-8 Et₃N
SOL 71-43-2 Benzene
CON room temperature

STAGE(2)

RCT J 106-49-0
SOL 64-19-7 AcOH
CON 4 hours, reflux

PRO K 22316-59-2

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

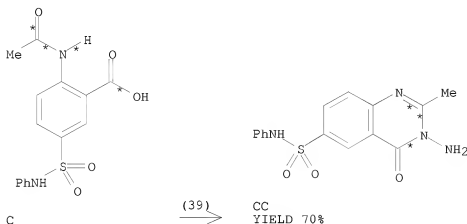
L3 ANSWER 66 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:350117 CASREACT

TITLE: Synthesis of 5-arylamino-sulpho-N-acetylanthranilic acid, 6-arylamino-sulpho-2-methyl-3-amino/3-N-chloroacetamido/3-N-arylamino

acetamido-4-(3H)-quinazolones as potential anti-HIV, anticancer and antimicrobial agents
 AUTHOR(S): Purohit, D. M.; Bhuva, V. R.; Shah, V. H.
 CORPORATE SOURCE: Department of Chemistry, Saurashtra University, Rajkot, 360 005, India
 SOURCE: Chemistry (Rajkot, India) (2003), 1(4), 233-245
 CODEN: CHEMCT; ISSN: 0972-8376
 PUBLISHER: Trade Science Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 5-Arylaminosulfo-N-acetylanthranilic acids, 3-amino-2-methyl-6-arylaminosulfo-4-(3H)-quinazalone, 3-N-(chloroacetamido)-2-methyl-6-arylaminosulpho-4-(3H)-quinazolones, 3-N-(arylaminoacetamido)-2-2 methyl-6-arylaminosulfo-4-(3H)-quinazolones have been synthesized. The products have been assayed for their anti-HIV activity, some of the products showed moderate activity in comparison to standard drug AZT. Anticancer activity were tested at five different concentration against 60 cell lines of human for nine types of cancers. Some of the compds. gave less activity as compare to 5-fluorodeoxyuridine (Standard drug). The products have been also evaluated for their antimicrobial activity by cup - plate method. Some of the compds. showed comparable antimicrobial activity with known antibiotics viz. Ampicillin, chloramphenicol, Norfloxacin and Griseofulvin. The constitution of the products have been delineated by IR, PMR, Mass spectral study and elemental analyses.

RX(39) OF 372 ...C ==> CC...



RX(39) RCT C 774216-86-3

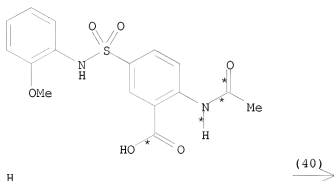
STAGE(1)
 RGT CD 7803-57-8 N2H4-H2O
 SOL 67-56-1 MeOH
 CON 3 hours, reflux

STAGE(2)
 RGT D 7732-18-5 Water
 CON cooled

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PRO CC 774217-23-1
NTE chemoselective

RX(40) OF 372 ...H ==> CF...



CF
YIELD 72%

RX(40) RCT H 774216-87-4

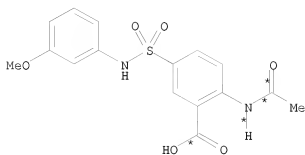
STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CF 774217-24-2
NTE chemoselective

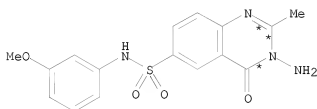
RX(41) OF 372 ...J ==> CG...

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J

(41)



CG

YIELD 75%

RX(41) RCT J 774216-88-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

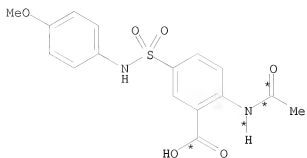
CON cooled

PRO CG 774217-25-3

NTE chemoselective

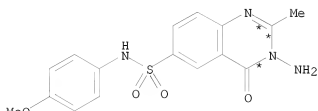
RX(42) OF 372 ...L ==> CH...

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L

(42)



CH

YIELD 73%

RX(42) RCT L 774216-89-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

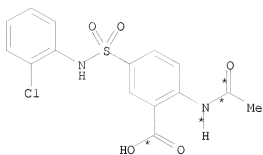
CON cooled

PRO CH 774217-26-4

NTE chemoselective

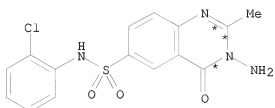
RX(43) OF 372 ...N ==> Cl...

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N

(43) \longrightarrow



CI
YIELD 65%

RX(43) RCT N 774216-90-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

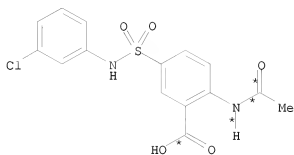
CON cooled

PRO CI 774217-27-5

NTE chemoselective

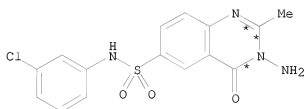
RX(44) OF 372 ...P ==> CJ...

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P

(44)



CJ
YIELD 68%

RX(44) RCT P 774216-91-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

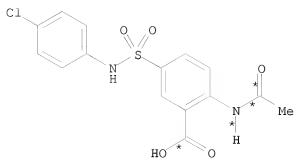
CON cooled

PRO CJ 774217-28-6

NTE chemoselective

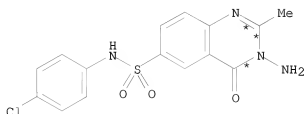
RX(45) OF 372 ...R ==> CK...

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R

(45) 



CK

YIELD 68%

RX(45) RCT R 774216-92-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

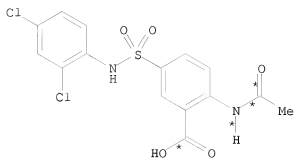
CON cooled

PRO CK 774217-29-7

NTE chemoselective

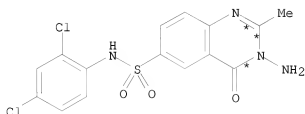
RX(46) OF 372 ...T ==> CL...

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T

(46)



CL
YIELD 72%

RX(46) RCT T 774216-93-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

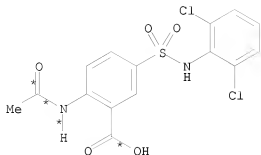
CON cooled

PRO CL 774217-30-0

NTE chemoselective

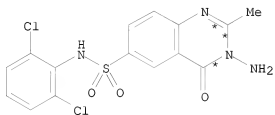
RX(47) OF 372 ...V ==> CM...

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V

(47) \longrightarrow



CM

YIELD 68%

RX(47) RCT V 774216-94-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

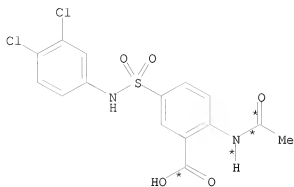
RGT D 7732-18-5 Water

CON cooled

PRO CM 774217-31-1

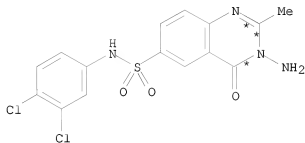
NTE chemoselective

RX(48) OF 372 ...X ==> CN...



X

(48)



CN

YIELD 72%

RX(48) RCT X 774216-95-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

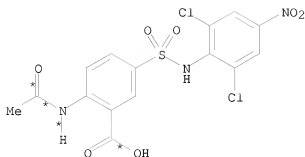
CON cooled

PRO CN 774217-32-2

NTE chemoselective

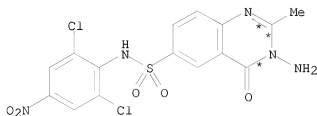
RX(49) OF 372 ...Z ==> CO...

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Z

(49)



CO

YIELD 81%

RX(49) RCT Z 218617-81-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

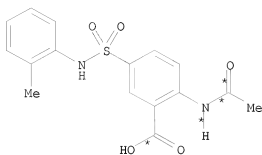
CON cooled

PRO CO 234096-58-3

NTE chemoselective

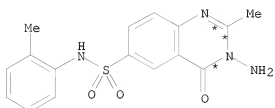
RX(50) OF 372 ...AB ==> CP...

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AB

(50) \longrightarrow



CP

YIELD 72%

RX(50) RCT AB 774216-96-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

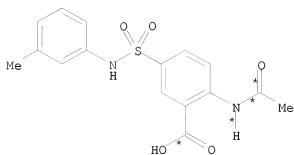
CON cooled

PRO CP 774217-33-3

NTE chemoselective

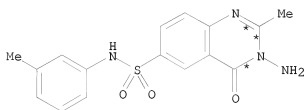
RX(51) OF 372 ...AD ==> CQ...

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AD

(51)



CQ

YIELD 74%

RX(51) RCT AD 774216-97-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

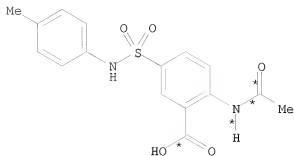
CON cooled

PRO CQ 774217-34-4

NTE chemoselective

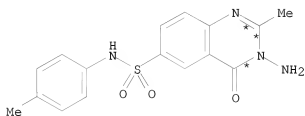
RX(52) OF 372 ...AF ==> CR...

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AF

(52) →



CR

YIELD 70%

RX(52) RCT AF 774216-98-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

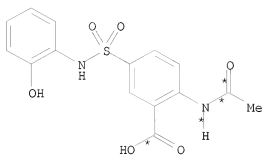
CON cooled

PRO CR 774217-35-5

NTE chemoselective

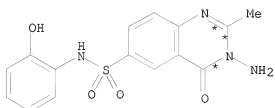
RX(53) OF 372 ...AH ==> CS...

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AH

(53) \longrightarrow



CS

YIELD 76%

RX(53) RCT AH 774216-99-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

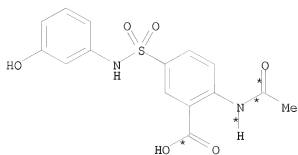
CON cooled

PRO CS 774217-36-6

NTE chemoselective

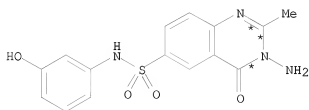
RX(54) OF 372 ...AJ ==> CT...

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AJ

(54) 



CT
YIELD 76%

RX(54) RCT AJ 774217-00-4

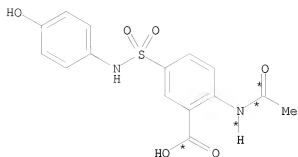
STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CT 774217-37-7
NTE chemoselective

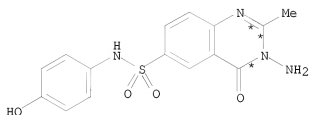
RX(55) OF 372 ...AL ==> CU...

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AL

(55)



CU

YIELD 72%

RX(55) RCT AL 774217-01-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

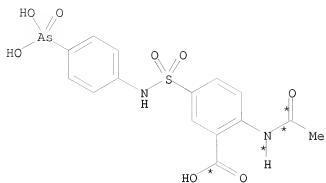
CON cooled

PRO CU 774217-38-8

NTE chemoselective

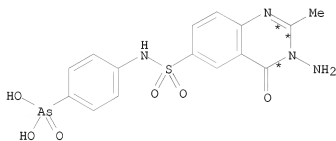
RX(56) OF 372 ...AN ==> CV...

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AN

(56)



CV

YIELD 81%

RX(56) RCT AN 774217-02-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

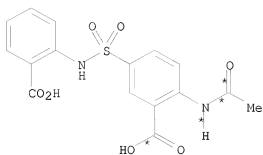
CON cooled

PRO CV 774217-39-9

NTE chemoselective

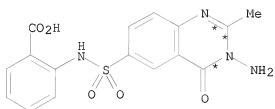
RX(57) OF 372 ...AP ==> CW...

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AP

(57) \longrightarrow



CW

YIELD 81%

RX(57) RCT AP 774217-03-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

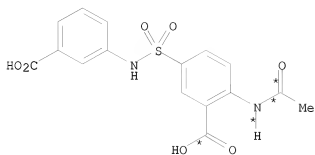
CON cooled

PRO CW 774217-40-2

NTE chemoselective

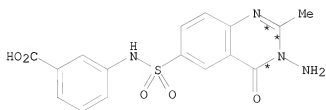
RX(58) OF 372 ...AR ==> CX...

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AR

(58)



CX

YIELD 82%

RX(58) RCT AR 774217-04-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

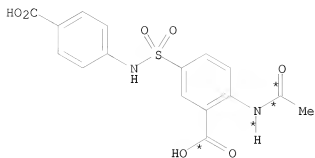
CON cooled

PRO CX 774217-41-3

NTE chemoselective

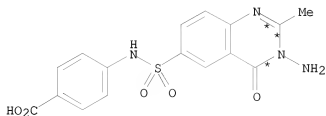
RX(59) OF 372 ...AT ==> CY...

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AT

(59) 



CY

YIELD 81%

RX(59) RCT AT 774217-05-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

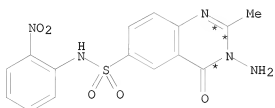
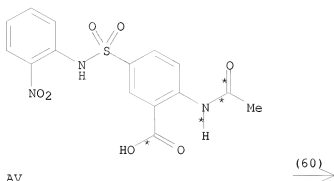
CON cooled

PRO CY 774217-42-4

NTE chemoselective

RX(60) OF 372 ...AV ==> CZ...

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CZ
YIELD 78%

RX(60) RCT AV 774217-06-0

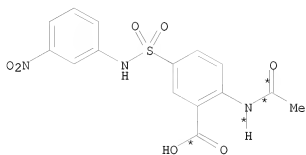
STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CZ 774217-43-5
NTE chemoselective

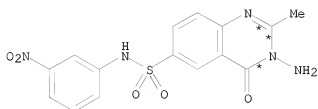
RX(61) OF 372 ...AX ==> DA...

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AX

(61)



DA

YIELD 76%

RX(61) RCT AX 774217-07-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

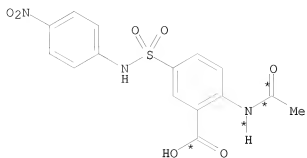
CON cooled

PRO DA 774217-44-6

NTE chemoselective

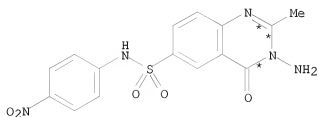
RX(62) OF 372 ...AZ ==> DB...

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AZ

(62)



DB

YIELD 79%

RX(62) RCT AZ 774217-08-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

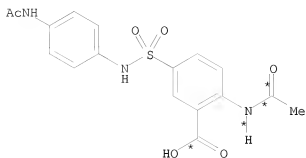
CON cooled

PRO DB 774217-45-7

NTE chemoselective

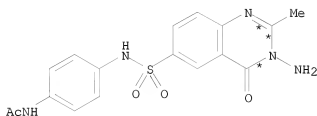
RX(63) OF 372 ...BB ==> DC...

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BB

(63)



DC

YIELD 71%

RX(63) RCT BB 774217-09-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

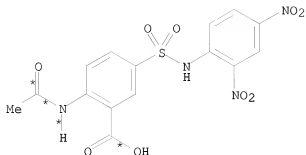
CON cooled

PRO DC 774217-46-8

NTE chemoselective

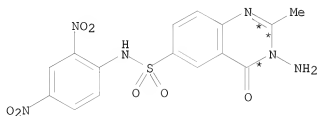
RX(64) OF 372 ...BD ==> DD...

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BD

(64)



DD

YIELD 76%

RX(64) RCT BD 774217-10-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

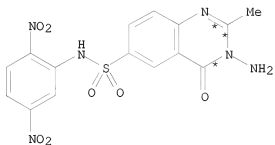
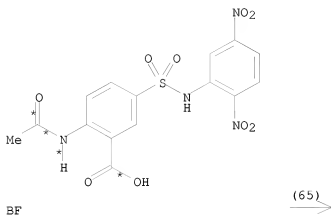
RGT D 7732-18-5 Water

CON cooled

PRO DD 774217-47-9

NTE chemoselective

RX(65) OF 372 ...BF ==> DE...



DE
YIELD 78%

RX(65) RCT BF 774217-11-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

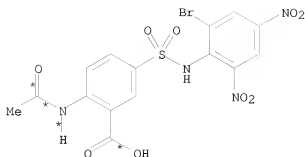
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DE 774217-48-0
NTE chemoselective

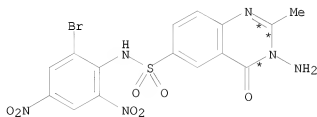
RX(66) OF 372 ...BH ==> DF...

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BH

(66) \longrightarrow



DF

YIELD 72%

RX(66) RCT BH 774217-12-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

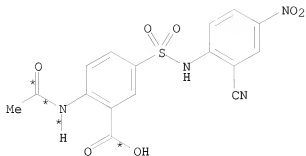
CON cooled

PRO DF 774217-49-1

NTE chemoselective

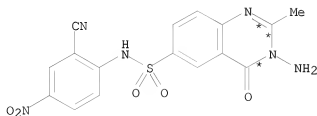
RX(67) OF 372 ...BJ ==> DG...

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BJ

(67)



DG

YIELD 71%

RX(67) RCT BJ 774217-13-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

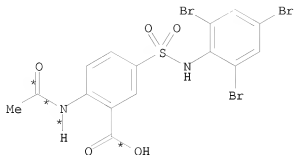
CON cooled

PRO DG 774217-50-4

NTE chemoselective

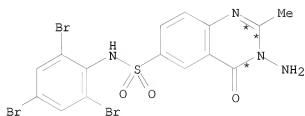
RX(68) OF 372 ...BL ==> DH...

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BL

(68)



DH

YIELD 80%

RX(68) RCT BL 774217-14-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

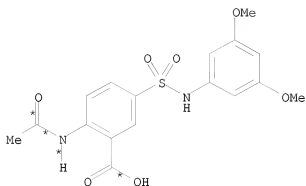
CON cooled

PRO DH 774217-51-5

NTE chemoselective

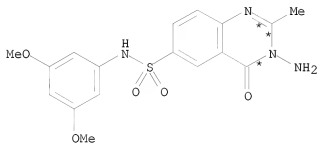
RX(69) OF 372 ...BN ==> DI...

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BN

(69)



DI

YIELD 75%

RX(69) RCT BN 774217-15-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

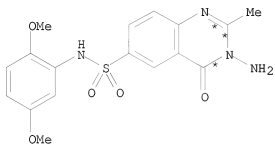
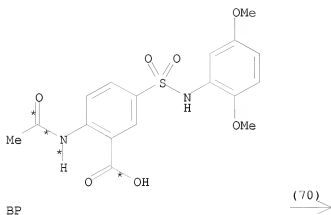
CON cooled

PRO DI 774217-52-6

NTE chemoselective

RX(70) OF 372 ...BP ==> DJ...

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DJ
YIELD 72%

RX(70) RCT BP 774217-16-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

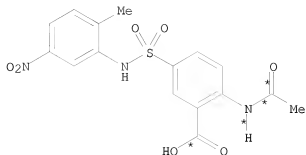
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DJ 774217-53-7
NTE chemoselective

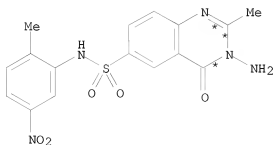
RX(71) OF 372 ...BR ==> DK...

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BR

(71) →



DK

YIELD 68%

RX(71) RCT BR 774217-17-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

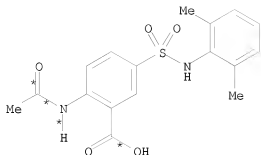
CON cooled

PRO DK 774217-54-8

NTE chemoselective

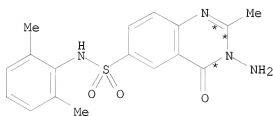
RX(72) OF 372 ...BV ==> DL...

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BV

(72)



DL

YIELD 72%

RX(72) RCT BV 774217-19-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

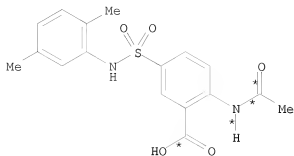
CON cooled

PRO DL 774217-56-0

NTE chemoselective

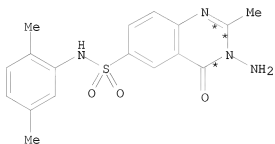
RX(73) OF 372 ...BX ==> DM...

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BX

(73)



DM

YIELD 70%

RX(73) RCT BX 774217-20-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

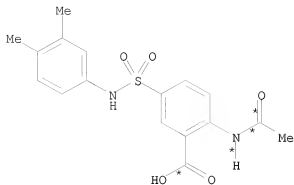
CON cooled

PRO DM 774217-57-1

NTE chemoselective

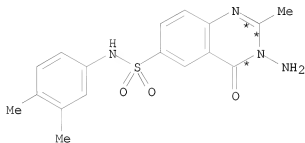
RX(74) OF 372 ...BZ ==> DN...

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BZ

(74) →



DN

YIELD 75%

RX(74) RCT BZ 774217-21-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

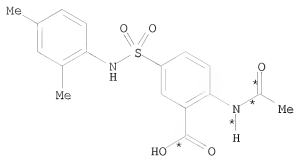
CON cooled

PRO DN 774217-58-2

NTE chemoselective

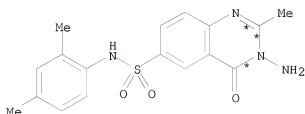
RX(75) OF 372 ...CB ==> DO...

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CB

(75) \longrightarrow



DO

YIELD 77%

RX(75) RCT CB 774217-22-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

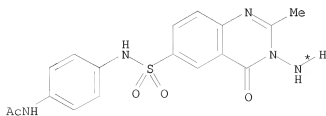
RGT D 7732-18-5 Water

CON cooled

PRO DO 774217-59-3

NTE chemoselective

RX(100) OF 372 ...DC + DP ==> EO...



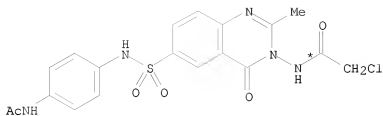
DC



DP

(100) \longrightarrow

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EO

YIELD 53%

RX(100) RCT DC 774217-46-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

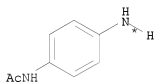
STAGE(2)

RGT D 7732-18-5 Water

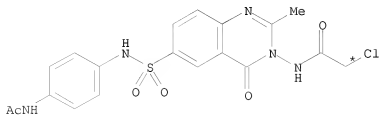
CON cooled

PRO EO 774217-84-4

RX(137) OF 372 ...BA + EO ==> FZ



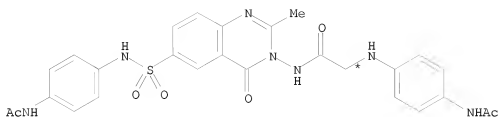
BA



EO

(137) \longrightarrow

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FZ
YIELD 53%

RX(137) RCT BA 122-80-5, EO 774217-84-4

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

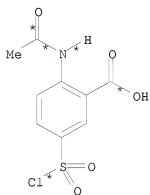
RGT D 7732-18-5 Water

CON cooled

PRO FZ 774218-18-7

RX(151) OF 372 COMPOSED OF RX(1), RX(39)

RX(151) A + B ==> CC



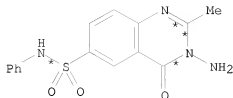
A



B

2
STEPS
→

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CC

YIELD 70%

RX(1) RCT A 181478-44-4, B 62-53-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO C 774216-86-3

RX(39) RCT C 774216-86-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

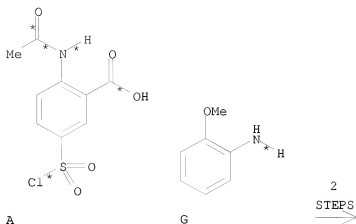
CON cooled

PRO CC 774217-23-1

NTE chemoselective

RX(152) OF 372 COMPOSED OF RX(2), RX(40)

RX(152) A + G ==> CF



CF
YIELD 72%

RX(2) RCT A 181478-44-4, G 90-04-0

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO H 774216-87-4

RX(40) RCT H 774216-87-4

STAGE(1)

RGT CD 7803-57-8 $\text{N}_2\text{H}_4\text{-H}_2\text{O}$
SOL 67-56-1 MeOH
CON 3 hours, reflux

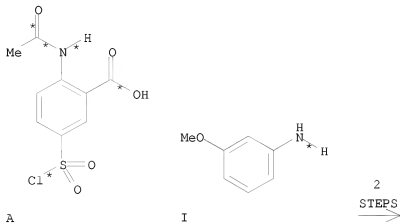
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

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PRO CF 774217-24-2
NTE chemoselective

RX(153) OF 372 COMPOSED OF RX(3), RX(41)
RX(153) A + I ==> CG



CG
YIELD 75%

RX(3) RCT A 181478-44-4, I 536-90-3

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO J 774216-88-5

RX(41) RCT J 774216-88-5

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O

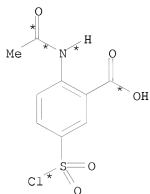
10/ 562,112

SOL 67-56-1 MeOH
CON 3 hours, reflux

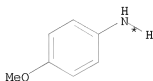
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CG 774217-25-3
NTE chemoselective

RX(154) OF 372 COMPOSED OF RX(4), RX(42)
RX(154) A + K ==> CH

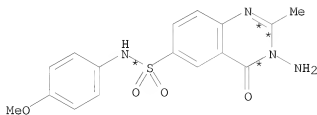


A



K

2
STEPS
→



CH

YIELD 73%

RX(4) RCT A 181478-44-4, K 104-94-9

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

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PRO L 774216-89-6

RX(42) RCT L 774216-89-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

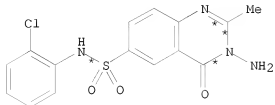
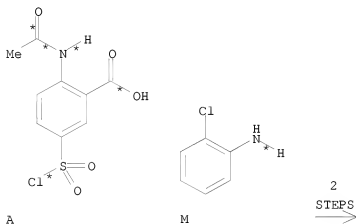
CON cooled

PRO CH 774217-26-4

NTE chemoselective

RX(155) OF 372 COMPOSED OF RX(5), RX(43)

RX(155) A + M ==> CI



CI

YIELD 65%

RX(5) RCT A 181478-44-4, M 95-51-2

STAGE(1)

CAT 110-86-1 Pyridine

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SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO N 774216-90-9

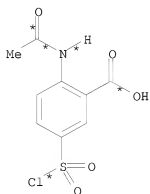
RX(43) RCT N 774216-90-9

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

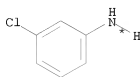
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CI 774217-27-5
NTE chemoselective

RX(156) OF 372 COMPOSED OF RX(6), RX(44)
RX(156) A + O ==> CJ

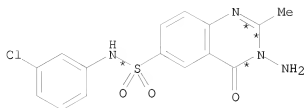


A



O

2
STEPS
→



CJ
YIELD 68%

RX(6) RCT A 181478-44-4, O 108-42-9

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO P 774216-91-0

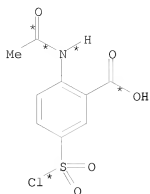
RX(44) RCT P 774216-91-0

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CJ 774217-28-6
NTE chemoselective

RX(157) OF 372 COMPOSED OF RX(7), RX(45)
RX(157) A + Q ==> CK

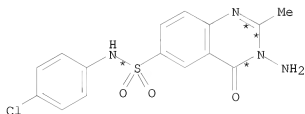


A



Q

2
STEPS
→



CK
YIELD 68%

RX(7) RCT A 181478-44-4, Q 106-47-8

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO R 774216-92-1

RX(45) RCT R 774216-92-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

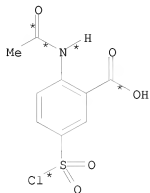
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

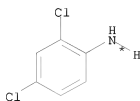
10/ 562,112

PRO CK 774217-29-7
NTE chemoselective

RX(158) OF 372 COMPOSED OF RX(8), RX(46)
RX(158) A + S ==> CL

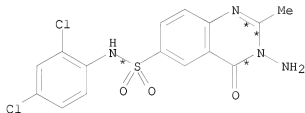


A



S

2
STEPS
→



CL
YIELD 72%

RX(8) RCT A 181478-44-4, S 554-00-7

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO T 774216-93-2

RX(46) RCT T 774216-93-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

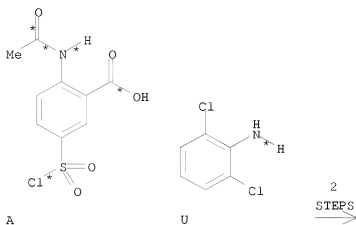
10/ 562,112

SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CL 774217-30-0
NTE chemoselective

RX(159) OF 372 COMPOSED OF RX(9), RX(47)
RX(159) A + U ==> CM



CM
YIELD 68%

RX(9) RCT A 181478-44-4, U 608-31-1

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

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PRO V 774216-94-3

RX(47) RCT V 774216-94-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

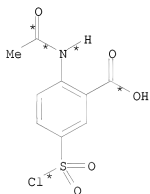
CON cooled

PRO CM 774217-31-1

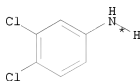
NTE chemoselective

RX(160) OF 372 COMPOSED OF RX(10), RX(48)

RX(160) A + W ==> CN

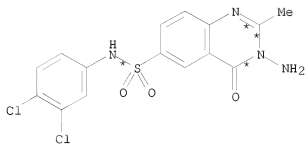


A



W

2
STEPS
→



CN

YIELD 72%

RX(10) RCT A 181478-44-4, W 95-76-1

STAGE(1)

CAT 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO X 774216-95-4

RX(48) RCT X 774216-95-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
 SOL 67-56-1 MeOH
 CON 3 hours, reflux

STAGE(2)

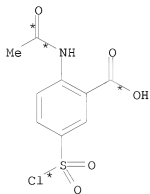
RGT D 7732-18-5 Water
 CON cooled

PRO CN 774217-32-2

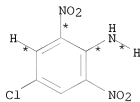
NIE chemoselective

RX(161) OF 372 COMPOSED OF RX(11), RX(49)

RX(161) A + Y ==> CO

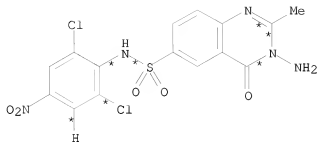


A



Y

2
 STEPS
 ➡



CO
YIELD 81%

RX(11) RCT A 181478-44-4, Y 5388-62-5

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO Z 218617-81-3

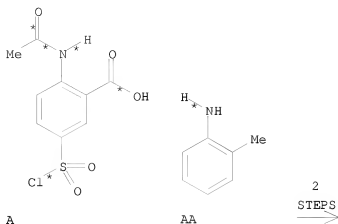
RX(49) RCT Z 218617-81-3

STAGE(1)
RGT CD 7803-57-8 N₂H₄-H₂O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CO 234096-58-3
NTE chemoselective

RX(162) OF 372 COMPOSED OF RX(12), RX(50)
RX(162) A + AA ==> CP



CP
YIELD 72%

RX(12) RCT A 181478-44-4, AA 95-53-4

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AB 774216-96-5

RX(50) RCT AB 774216-96-5

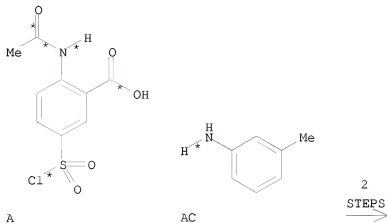
STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

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PRO CP 774217-33-3
NTE chemoselective

RX(163) OF 372 COMPOSED OF RX(13), RX(51)
RX(163) A + AC ==> CQ



CQ
YIELD 74%

RX(13) RCT A 181478-44-4, AC 108-44-1

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AD 774216-97-6

RX(51) RCT AD 774216-97-6

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O

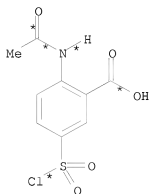
10/ 562,112

SOL 67-56-1 MeOH
CON 3 hours, reflux

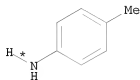
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CQ 774217-34-4
NTE chemoselective

RX(164) OF 372 COMPOSED OF RX(14), RX(52)
RX(164) A + AE ==> CR

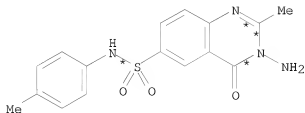


A



AE

2
STEPS
→



CR
YIELD 70%

RX(14) RCT A 181478-44-4, AE 106-49-0

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

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PRO AF 774216-98-7

RX(52) RCT AF 774216-98-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

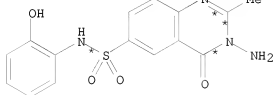
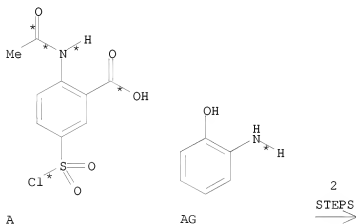
CON cooled

PRO CR 774217-35-5

NTE chemoselective

RX(165) OF 372 COMPOSED OF RX(15), RX(53)

RX(165) A + AG ==> CS



CS

YIELD 76%

RX(15) RCT A 181478-44-4, AG 95-55-6

STAGE(1)

CAT 110-86-1 Pyridine

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SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AH 774216-99-8

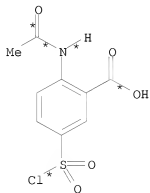
RX(53) RCT AH 774216-99-8

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

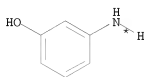
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CS 774217-36-6
NTE chemoselective

RX(166) OF 372 COMPOSED OF RX(16), RX(54)
RX(166) A + AI ==> CT

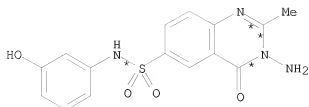


A



AI

2
STEPS
→



CT

YIELD 76%

RX(16) RCT A 181478-44-4, AI 591-27-5

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AJ 774217-00-4

RX(54) RCT AJ 774217-00-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

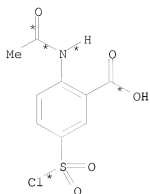
PRO CT 774217-37-7

NTE chemoselective

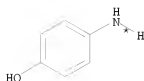
RX(167) OF 372 COMPOSED OF RX(17), RX(55)

RX(167) A + AK ==> CU

10/ 562,112

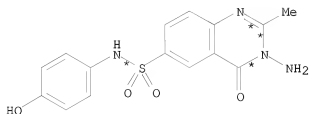


A



AK

2
STEPS
→



CU

YIELD 72%

RX(17) RCT A 181478-44-4, AK 123-30-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AL 774217-01-5

RX(55) RCT AL 774217-01-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

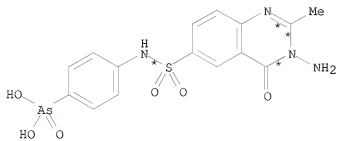
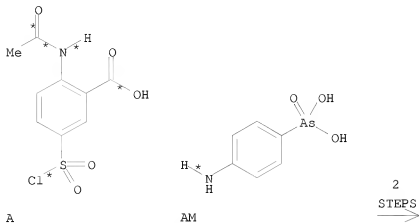
RGT D 7732-18-5 Water

CON cooled

10/ 562,112

PRO CU 774217-38-8
NTE chemoselective

RX(168) OF 372 COMPOSED OF RX(18), RX(56)
RX(168) A + AM ==> CV



CV
YIELD 81%

RX(18) RCT A 181478-44-4, AM 98-50-0

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AN 774217-02-6

RX(56) RCT AN 774217-02-6

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STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

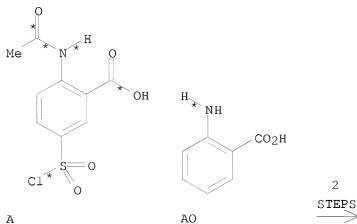
CON cooled

PRO CV 774217-39-9

NTE chemoselective

RX(169) OF 372 COMPOSED OF RX(19), RX(57)

RX(169) A + AO ==> CW



CW
YIELD 81%

RX(19) RCT A 181478-44-4, AO 118-92-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

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RGT D 7732-18-5 Water
CON cooled

PRO AP 774217-03-7

RX(57) RCT AP 774217-03-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

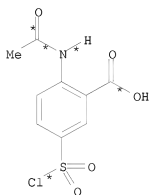
RGT D 7732-18-5 Water
CON cooled

PRO CW 774217-40-2

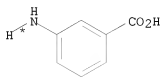
NTE chemoselective

RX(170) OF 372 COMPOSED OF RX(20), RX(58)

RX(170) A + AQ ==> CX

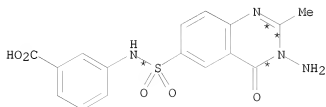


A



AQ

2
STEPS
→



CX

YIELD 82%

RX(20) RCT A 181478-44-4, AQ 99-05-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AR 774217-04-8

RX(58) RCT AR 774217-04-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

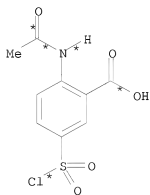
CON cooled

PRO CX 774217-41-3

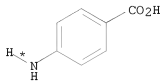
NTE chemoselective

RX(171) OF 372 COMPOSED OF RX(21), RX(59)

RX(171) A + AS ==> CY

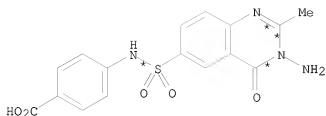


A



AS

2
STEPS
→



CY
YIELD 81%

RX(21) RCT A 181478-44-4, AS 150-13-0

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AT 774217-05-9

RX(59) RCT AT 774217-05-9

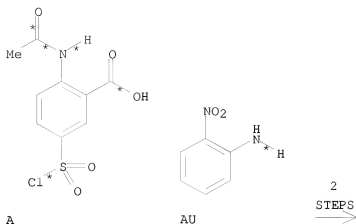
STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CY 774217-42-4
NTE chemoselective

RX(172) OF 372 COMPOSED OF RX(22), RX(60)

RX(172) A + AU ==> CZ



CZ
YIELD 78%

RX(22) RCT A 181478-44-4, AU 88-74-4

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO AV 774217-06-0

RX(60) RCT AV 774217-06-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

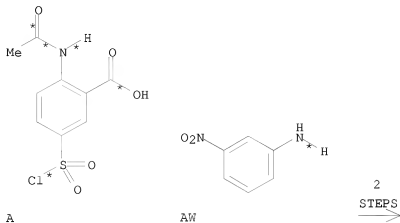
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

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PRO CZ 774217-43-5
NTE chemoselective

RX(173) OF 372 COMPOSED OF RX(23), RX(61)
RX(173) A + AW ==> DA



DA
YIELD 76%

RX(23) RCT A 181478-44-4, AW 99-09-2

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO AX 774217-07-1

RX(61) RCT AX 774217-07-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

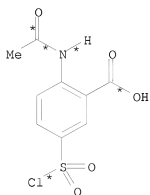
10/ 562,112

SOL 67-56-1 MeOH
CON 3 hours, reflux

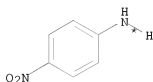
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DA 774217-44-6
NTE chemoselective

RX(174) OF 372 COMPOSED OF RX(24), RX(62)
RX(174) A + AY ==> DB

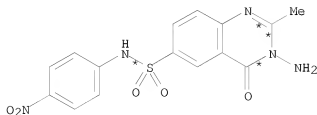


A



AY

2
STEPS
→



DB
YIELD 79%

RX(24) RCT A 181478-44-4, AY 100-01-6

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

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PRO AZ 774217-08-2

RX(62) RCT AZ 774217-08-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

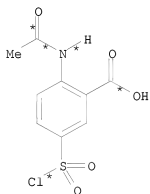
CON cooled

PRO DB 774217-45-7

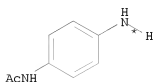
NIE chemoselective

RX(175) OF 372 COMPOSED OF RX(25), RX(63)

RX(175) A + BA ==> DC

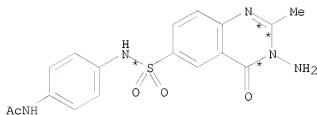


A



BA

2
STEPS
→



DC

YIELD 71%

RX(25) RCT A 181478-44-4, BA 122-80-5

STAGE(1)

CAT 110-86-1 Pyridine

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SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO BB 774217-09-3

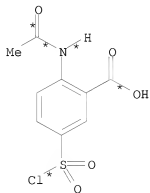
RX(63) RCT BB 774217-09-3

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

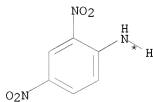
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DC 774217-46-8
NTE chemoselective

RX(176) OF 372 COMPOSED OF RX(26), RX(64)
RX(176) A + BC ==> DD

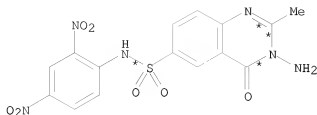


A



BC

2
STEPS
→



DD
YIELD 76%

RX(26) RCT A 181478-44-4, BC 97-02-9

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BD 774217-10-6

RX(64) RCT BD 774217-10-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

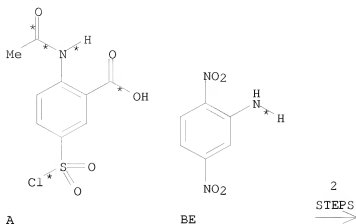
RGT D 7732-18-5 Water
CON cooled

PRO DD 774217-47-9

NTE chemoselective

RX(177) OF 372 COMPOSED OF RX(27), RX(65)

RX(177) A + BE ==> DE



DE
YIELD 78%

RX(27) RCT A 181478-44-4, BE 619-18-1

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BF 774217-11-7

RX(65) RCT BF 774217-11-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

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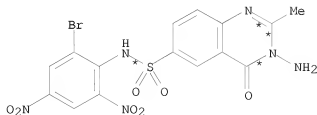
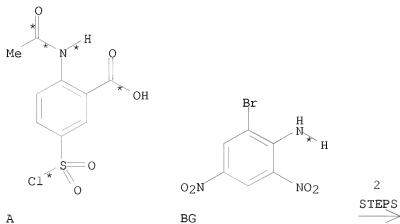
CON cooled

PRO DE 774217-48-0

NTE chemoselective

RX(178) OF 372 COMPOSED OF RX(28), RX(66)

RX(178) A + BG ==> DF



DF
YIELD 72%

RX(28) RCT A 181478-44-4, BG 1817-73-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BH 774217-12-8

RX(66) RCT BH 774217-12-8

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STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

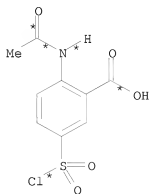
CON cooled

PRO DF 774217-49-1

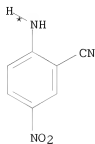
NTE chemoselective

RX(179) OF 372 COMPOSED OF RX(29), RX(67)

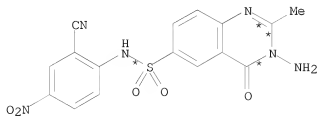
RX(179) A + BI ==> DG



A



BI



DG

YIELD 71%

RX(29) RCT A 181478-44-4, BI 17420-30-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

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RGT D 7732-18-5 Water
CON cooled

PRO BJ 774217-13-9

RX(67) RCT BJ 774217-13-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

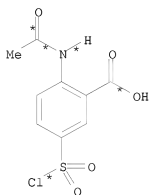
RGT D 7732-18-5 Water
CON cooled

PRO DG 774217-50-4

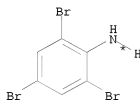
NTE chemoselective

RX(180) OF 372 COMPOSED OF RX(30), RX(68)

RX(180) A + BK ==> DH

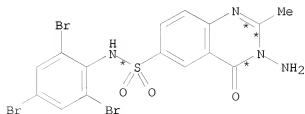


A



BK

2
STEPS
→



DH

YIELD 80%

RX(30) RCT A 181478-44-4, BK 147-82-0

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BL 774217-14-0

RX(68) RCT BL 774217-14-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

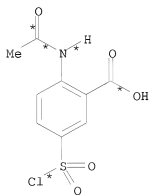
CON cooled

PRO DH 774217-51-5

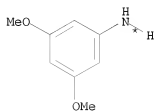
NIE chemoselective

RX(181) OF 372 COMPOSED OF RX(31), RX(69)

RX(181) A + BM ==> DI



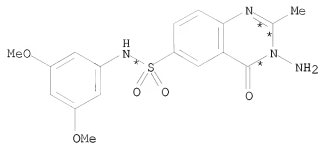
A



BM

2
STEPS
→

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DI
YIELD 75%

RX(31) RCT A 181478-44-4, BM 10272-07-8

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BN 774217-15-1

RX(69) RCT BN 774217-15-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

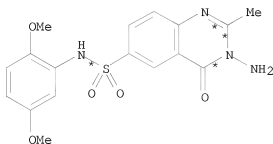
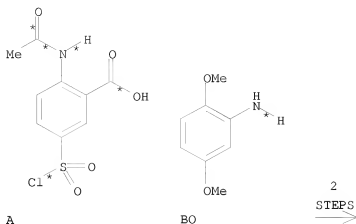
RGT D 7732-18-5 Water
CON cooled

PRO DI 774217-52-6

NTE chemoselective

RX(182) OF 372 COMPOSED OF RX(32), RX(70)

RX(182) A + BO ==> DJ



DJ
YIELD 72%

RX(32) RCT A 181478-44-4, BO 102-56-7

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO BP 774217-16-2

RX(70) RCT BP 774217-16-2

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water

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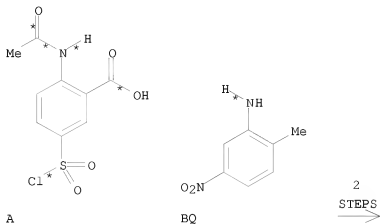
CON cooled

PRO DJ 774217-53-7

NTE chemoselective

RX(183) OF 372 COMPOSED OF RX(33), RX(71)

RX(183) A + BQ ==> DK



DK
YIELD 68%

RX(33) RCT A 181478-44-4, BQ 99-55-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BR 774217-17-3

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RX(71) RCT BR 774217-17-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

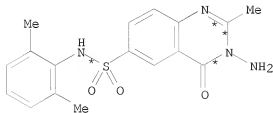
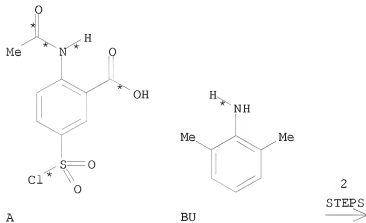
CON cooled

PRO DK 774217-54-8

NTE chemoselective

RX(184) OF 372 COMPOSED OF RX(35), RX(72)

RX(184) A + BU ==> DL



DL
YIELD 72%

RX(35) RCT A 181478-44-4, BU 87-62-7

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

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STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BV 774217-19-5

RX(72) RCT BV 774217-19-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

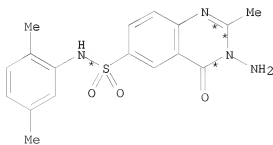
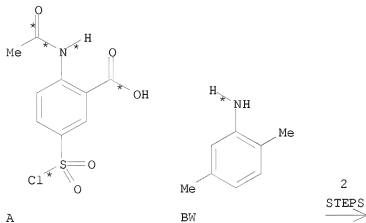
RGT D 7732-18-5 Water
CON cooled

PRO DL 774217-56-0

NTE chemoselective

RX(185) OF 372 COMPOSED OF RX(36), RX(73)

RX(185) A + BW ==> DM



DM
YIELD 70%

RX(36) RCT A 181478-44-4, BW 95-78-3

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BX 774217-20-8

RX(73) RCT BX 774217-20-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

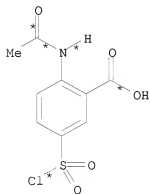
RGT D 7732-18-5 Water
CON cooled

PRO DM 774217-57-1

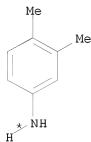
NTE chemoselective

RX(186) OF 372 COMPOSED OF RX(37), RX(74)

RX(186) A + BY ==> DN

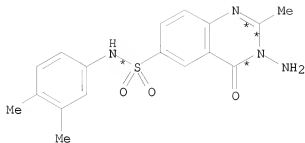


A



BY

2
STEPS
→



DN
YIELD 75%

RX(37) RCT A 181478-44-4, BY 95-64-7

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BZ 774217-21-9

RX(74) RCT BZ 774217-21-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

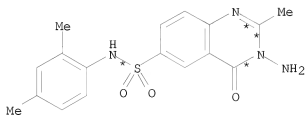
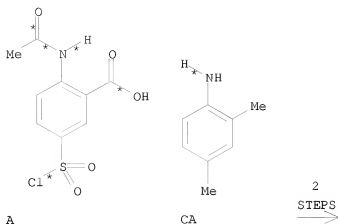
RGT D 7732-18-5 Water
CON cooled

PRO DN 774217-58-2

NTE chemoselective

RX(187) OF 372 COMPOSED OF RX(38), RX(75)

RX(187) A + CA ==> DO



DO
YIELD 77%

RX(38) RCT A 181478-44-4, CA 95-68-1

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CB 774217-22-0

RX(75) RCT CB 774217-22-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

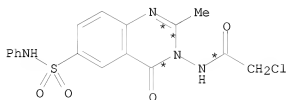
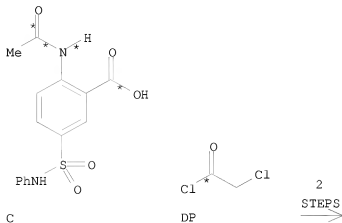
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

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PRO DO 774217-59-3
NTE chemoselective

RX(188) OF 372 COMPOSED OF RX(39), RX(76)
RX(188) C + DP ==> DQ



DQ
YIELD 61%

RX(39) RCT C 774216-86-3

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CC 774217-23-1
NTE chemoselective

RX(76) RCT CC 774217-23-1, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

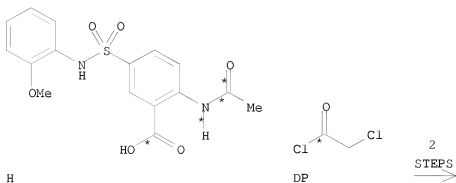
RGT D 7732-18-5 Water

CON cooled

PRO DQ 774217-60-6

RX(189) OF 372 COMPOSED OF RX(40), RX(77)

RX(189) H + DP ==> DR



DR
YIELD 59%

RX(40) RCT H 774216-87-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CF 774217-24-2

NTE chemoselective

RX(77) RCT CF 774217-24-2, DP 79-04-9

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STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

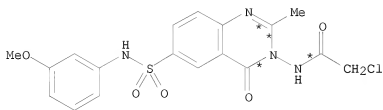
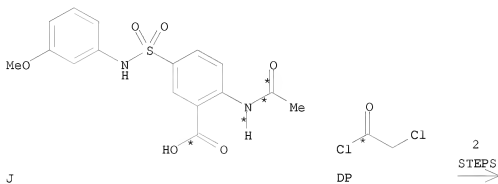
RGT D 7732-18-5 Water

CON cooled

PRO DR 774217-61-7

RX(190) OF 372 COMPOSED OF RX(41), RX(78)

RX(190) J + DP ==> DS



DS

YIELD 53%

RX(41) RCT J 774216-88-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CG 774217-25-3

NTE chemoselective

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RX(78) RCT CG 774217-25-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

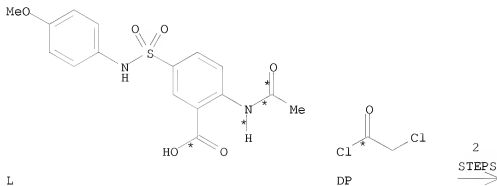
RGT D 7732-18-5 Water

CON cooled

PRO DS 774217-62-8

RX(191) OF 372 COMPOSED OF RX(42), RX(79)

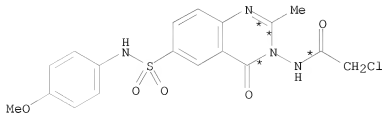
RX(191) L + DP ==> DT



L

DP

2
STEPS
→



DT
YIELD 63%

RX(42) RCT L 774216-89-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

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PRO CH 774217-26-4
NTE chemoselective

RX(79) RCT CH 774217-26-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

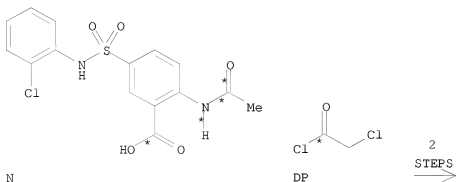
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DT 774217-63-9

RX(192) OF 372 COMPOSED OF RX(43), RX(80)

RX(192) N + DP ==> DU



DU
YIELD 53%

RX(43) RCT N 774216-90-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

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STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CI 774217-27-5
NTE chemoselective

RX(80) RCT CI 774217-27-5, DP 79-04-9

STAGE(1)

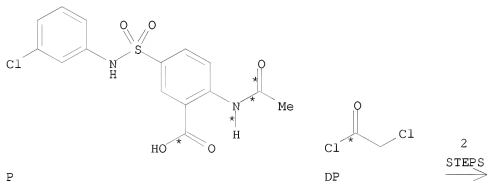
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DU 774217-64-0

RX(193) OF 372 COMPOSED OF RX(44), RX(81)
RX(193) P + DP ==> DV



DV
YIELD 59%

RX(44) RCT P 774216-91-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

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SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CJ 774217-28-6
NTE chemoselective

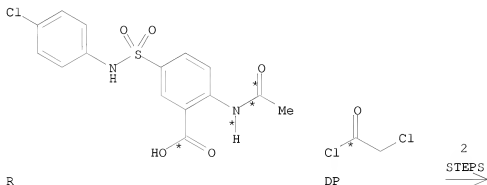
RX(81) RCT CJ 774217-28-6, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

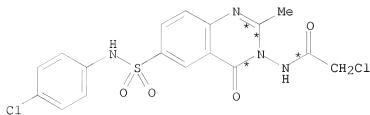
PRO DV 774217-65-1

RX(194) OF 372 COMPOSED OF RX(45), RX(82)
RX(194) R + DP ==> DW



R

DP



DW
YIELD 58%

RX(45) RCT R 774216-92-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CK 774217-29-7

NTE chemoselective

RX(82) RCT CK 774217-29-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

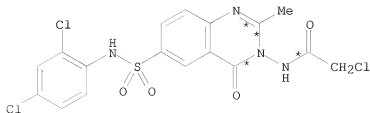
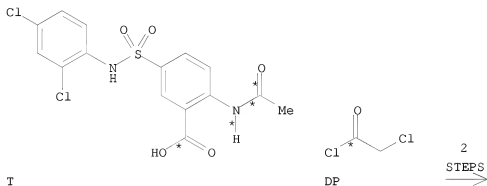
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DW 774217-66-2

RX(195) OF 372 COMPOSED OF RX(46), RX(83)

RX(195) T + DP ==> DX



DX
YIELD 63%

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RX(46) RCT T 774216-93-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CL 774217-30-0
NTE chemoselective

RX(83) RCT CL 774217-30-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

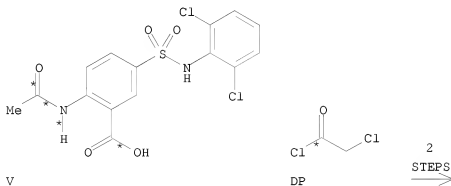
STAGE(2)

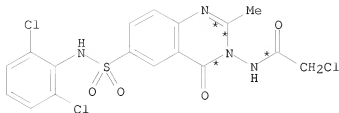
RGT D 7732-18-5 Water
CON cooled

PRO DX 774217-67-3

RX(196) OF 372 COMPOSED OF RX(47), RX(84)

RX(196) V + DP ==> DY





DY
YIELD 57%

RX(47) RCT V 774216-94-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CM 774217-31-1
NTE chemoselective

RX(84) RCT CM 774217-31-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

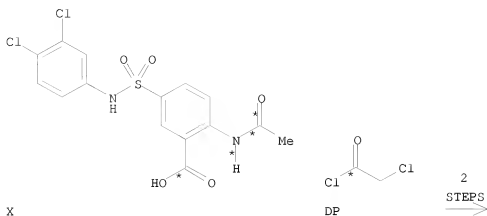
RGT D 7732-18-5 Water
CON cooled

PRO DY 774217-68-4

RX(197) OF 372 COMPOSED OF RX(48), RX(85)

RX(197) X + DP ==> DZ

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DZ
YIELD 57%

RX(48) RCT X 774216-95-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CN 774217-32-2
NTE chemoselective

RX(85) RCT CN 774217-32-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

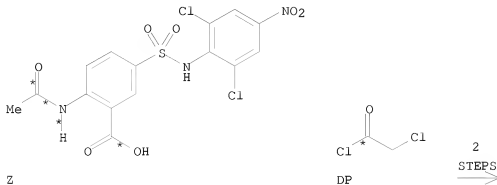
10/ 562,112

CON cooled

PRO DZ 774217-69-5

RX(198) OF 372 COMPOSED OF RX(49), RX(86)

RX(198) Z + DP ==> EA



EA

YIELD 62%

RX(49) RCT Z 218617-81-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CO 234096-58-3

NTE chemoselective

RX(86) RCT CO 234096-58-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

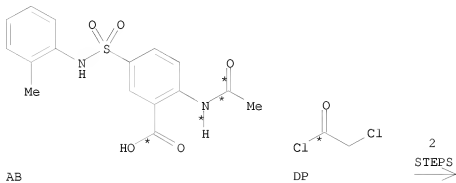
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STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EA 774217-70-8

RX(199) OF 372 COMPOSED OF RX(50), RX(87)
RX(199) AB + DP ==> EB



EB
YIELD 59%

RX(50) RCT AB 774216-96-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CP 774217-33-3
NTE chemoselective

RX(87) RCT CP 774217-33-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

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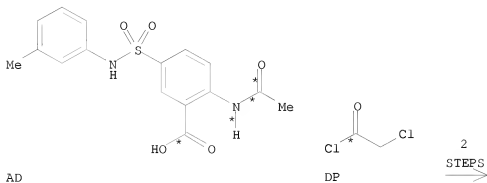
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EB 774217-71-9

RX(200) OF 372 COMPOSED OF RX(51), RX(88)
RX(200) AD + DP ==> EC



EC
YIELD 64%

RX(51) RCT AD 774216-97-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CQ 774217-34-4
NTE chemoselective

RX(88) RCT CQ 774217-34-4, DP 79-04-9

STAGE(1)

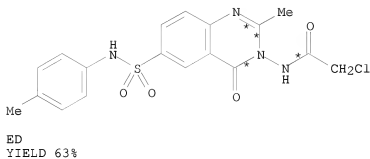
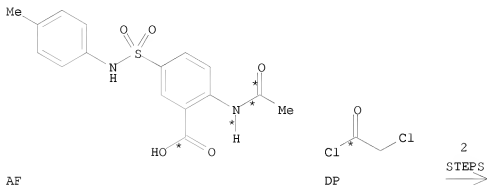
RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO EC 774217-72-0

RX(201) OF 372 COMPOSED OF RX(52), RX(89)
 RX(201) AF + DP ==> ED



RX(52) RCT AF 774216-98-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
 SOL 67-56-1 MeOH
 CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO CR 774217-35-5

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NTE chemoselective

RX(89) RCT CR 774217-35-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

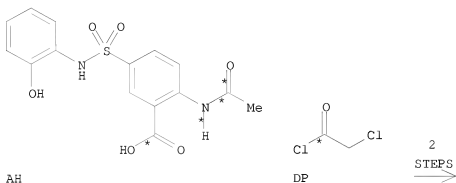
RGT D 7732-18-5 Water

CON cooled

PRO ED 774217-73-1

RX(202) OF 372 COMPOSED OF RX(53), RX(90)

RX(202) AH + DP ==> EE



EE
YIELD 58%

RX(53) RCT AH 774216-99-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

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CON cooled

PRO CS 774217-36-6
NTE chemoselective

RX(90) RCT CS 774217-36-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

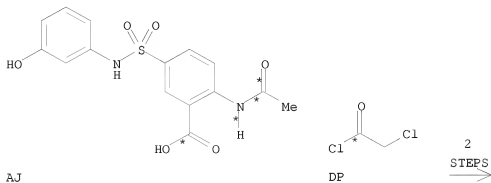
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EE 774217-74-2

RX(203) OF 372 COMPOSED OF RX(54), RX(91)

RX(203) AJ + DP ==> EF



EF
YIELD 59%

RX(54) RCT AJ 774217-00-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

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STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CT 774217-37-7

NTE chemoselective

RX(91) RCT CT 774217-37-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

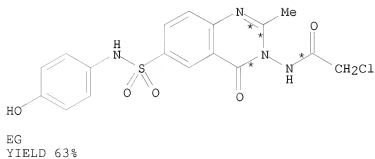
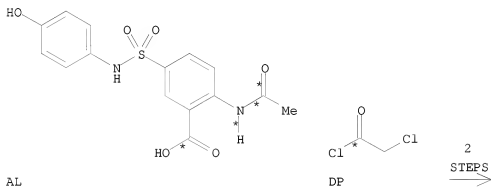
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EF 774217-75-3

RX(204) OF 372 COMPOSED OF RX(55), RX(92)

RX(204) AL + DP ==> EG



RX(55) RCT AL 774217-01-5

STAGE(1)

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RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CU 774217-38-8
NTE chemoselective

RX(92) RCT CU 774217-38-8, DP 79-04-9

STAGE(1)

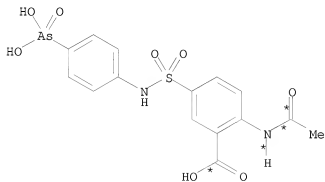
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EG 774217-76-4

RX(205) OF 372 COMPOSED OF RX(56), RX(93)
RX(205) AN + DP ==> EH

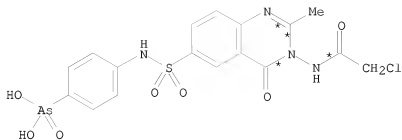


AN



DP

2
STEPS
→



EH

YIELD 71%

RX(56) RCT AN 774217-02-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CV 774217-39-9

NTE chemoselective

RX(93) RCT CV 774217-39-9, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

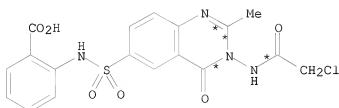
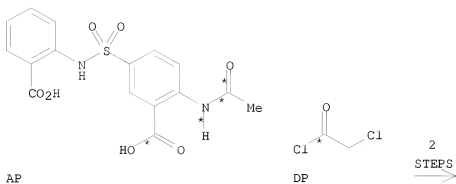
RGT D 7732-18-5 Water

CON cooled

PRO EH 774217-77-5

RX(206) OF 372 COMPOSED OF RX(57), RX(94)

RX(206) AP + DP ==> EI



EI
YIELD 75%

RX(57) RCT AP 774217-03-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CW 774217-40-2
NTE chemoselective

RX(94) RCT CW 774217-40-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

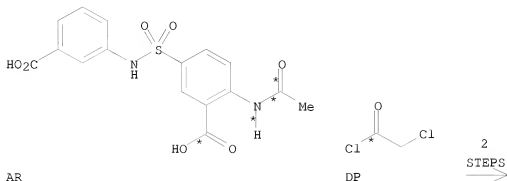
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EI 774217-78-6

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RX(207) OF 372 COMPOSED OF RX(58), RX(95)
RX(207) AR + DP ==> EJ



EJ
YIELD 70%

RX(58) RCT AR 774217-04-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CX 774217-41-3
NTE chemoselective

RX(95) RCT CX 774217-41-3, DP 79-04-9

STAGE(1)

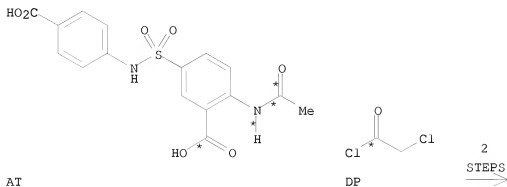
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EJ 774217-79-7

RX(208) OF 372 COMPOSED OF RX(59), RX(96)
 RX(208) AT + DP ==> EK



EK
 YIELD 68%

RX(59) RCT AT 774217-05-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
 SOL 67-56-1 MeOH
 CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO CY 774217-42-4
 NTE chemoselective

RX(96) RCT CY 774217-42-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

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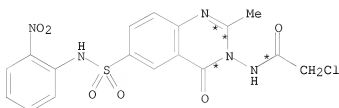
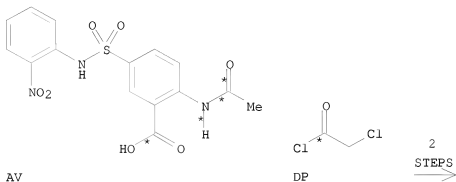
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EK 774217-80-0

RX(209) OF 372 COMPOSED OF RX(60), RX(97)

RX(209) AV + DP ==> EL



EL
YIELD 75%

RX(60) RCT AV 774217-06-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CZ 774217-43-5
NTE chemoselective

RX(97) RCT CZ 774217-43-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

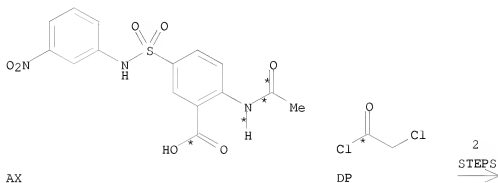
RGT D 7732-18-5 Water

CON cooled

PRO EL 774217-81-1

RX(210) OF 372 COMPOSED OF RX(61), RX(98)

RX(210) AX + DP ==> EM



EM

YIELD 78%

RX(61) RCT AX 774217-07-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DA 774217-44-6

NTE chemoselective

RX(98) RCT DA 774217-44-6, DP 79-04-9

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STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

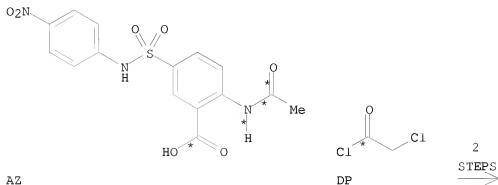
RGT D 7732-18-5 Water

CON cooled

PRO EM 774217-82-2

RX(211) OF 372 COMPOSED OF RX(62), RX(99)

RX(211) AZ + DP ==> EN



EN

YIELD 71%

RX(62) RCT AZ 774217-08-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DB 774217-45-7

NTE chemoselective

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RX(99) RCT DB 774217-45-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

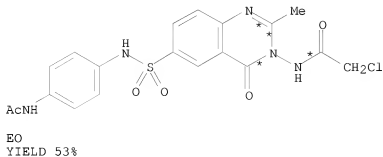
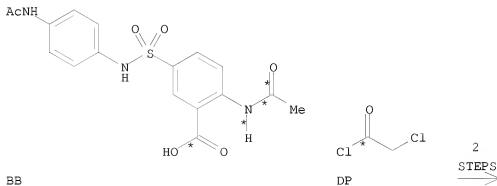
RGT D 7732-18-5 Water

CON cooled

PRO EN 774217-83-3

RX(212) OF 372 COMPOSED OF RX(63), RX(100)

RX(212) BB + DP ==> EO



RX(63) RCT BB 774217-09-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

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PRO DC 774217-46-8
NTE chemoselective

RX(100) RCT DC 774217-46-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

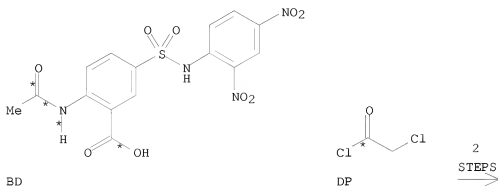
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EO 774217-84-4

RX(213) OF 372 COMPOSED OF RX(64), RX(101)

RX(213) BD + DP ==> EP



EP
YIELD 57%

RX(64) RCT BD 774217-10-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

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STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DD 774217-47-9
NTE chemoselective

RX(101) RCT DD 774217-47-9, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

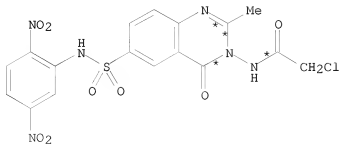
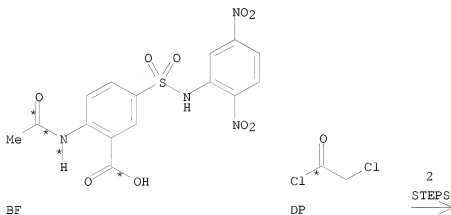
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EP 774217-85-5

RX(214) OF 372 COMPOSED OF RX(65), RX(102)

RX(214) BF + DP ==> EQ



EQ
YIELD 57%

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RX(65) RCT BF 774217-11-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DE 774217-48-0

NTE chemoselective

RX(102) RCT DE 774217-48-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

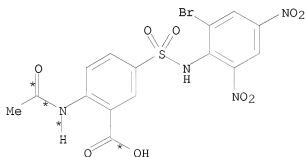
RGT D 7732-18-5 Water

CON cooled

PRO EQ 774217-86-6

RX(215) OF 372 COMPOSED OF RX(66), RX(103)

RX(215) BH + DP ==> ER



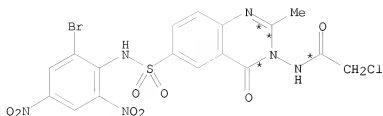
BH



DP

2
STEPS
→

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ER
YIELD 54%

RX(66) RCT BH 774217-12-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DF 774217-49-1
NTE chemoselective

RX(103) RCT DF 774217-49-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

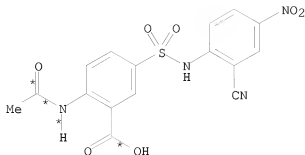
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO ER 774217-87-7

RX(216) OF 372 COMPOSED OF RX(67), RX(104)

RX(216) BJ + DP ==> ES

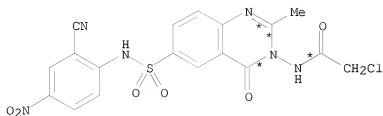


BJ



DP

2
STEPS
→



ES

YIELD 51%

RX(67) RCT BJ 774217-13-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DG 774217-50-4

NTE chemoselective

RX(104) RCT DG 774217-50-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

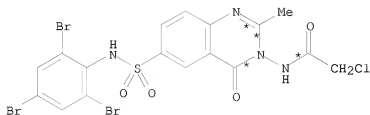
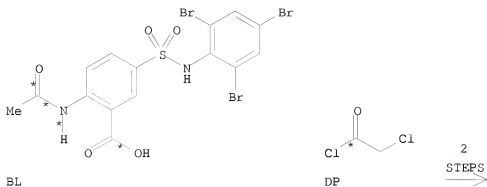
RGT D 7732-18-5 Water

CON cooled

PRO ES 774217-88-8

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RX(217) OF 372 COMPOSED OF RX(68), RX(105)
RX(217) BL + DP ==> ET



ET
YIELD 58%

RX(68) RCT BL 774217-14-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DH 774217-51-5

NTE chemoselective

RX(105) RCT DH 774217-51-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

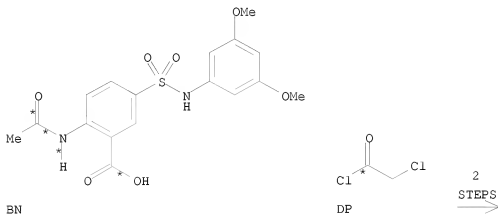
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO ET 774217-89-9

RX(218) OF 372 COMPOSED OF RX(69), RX(106)

RX(218) BN + DP ==> EU

EU
YIELD 63%

RX(69) RCT BN 774217-15-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DI 774217-52-6

NTE chemoselective

RX(106) RCT DI 774217-52-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

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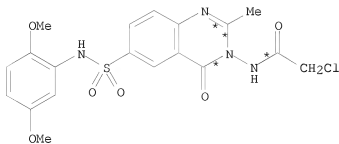
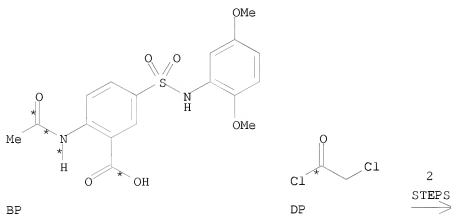
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EU 774217-90-2

RX(219) OF 372 COMPOSED OF RX(70), RX(107)
RX(219) BP + DP ==> EV



EV
YIELD 63%

RX(70) RCT BP 774217-16-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

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PRO DJ 774217-53-7
NTE chemoselective

RX(107) RCT DJ 774217-53-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

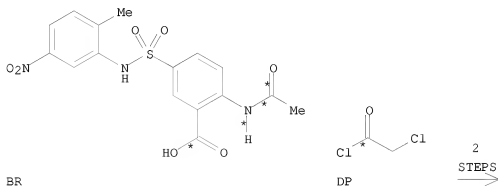
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EV 774217-91-3

RX(220) OF 372 COMPOSED OF RX(71), RX(108)

RX(220) BR + DP ==> EW



EW
YIELD 58%

RX(71) RCT BR 774217-17-3

STAGE(1)

RGT CD 7803-57-8 N₂H₄-H₂O
SOL 67-56-1 MeOH

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CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DK 774217-54-8

NTE chemoselective

RX(108) RCT DK 774217-54-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

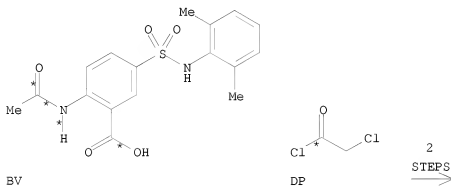
RGT D 7732-18-5 Water

CON cooled

PRO EW 774217-92-4

RX(221) OF 372 COMPOSED OF RX(72), RX(109)

RX(221) BV + DP ==> EX



EX

YIELD 56%

RX(72) RCT BV 774217-19-5

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STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DL 774217-56-0
NTE chemoselective

RX(109) RCT DL 774217-56-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

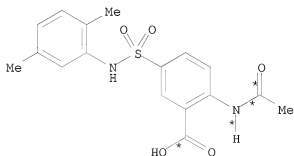
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EX 774217-94-6

RX(222) OF 372 COMPOSED OF RX(73), RX(110)

RX(222) BX + DP ==> EY

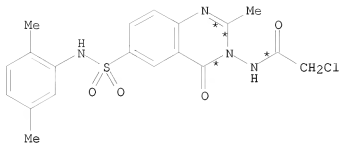


BX



DP

2
STEPS
→



EY
YIELD 59%

RX(73) RCT BX 774217-20-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DM 774217-57-1
NTE chemoselective

RX(110) RCT DM 774217-57-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

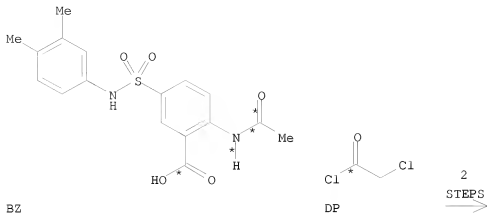
RGT D 7732-18-5 Water
CON cooled

PRO EY 774217-95-7

RX(223) OF 372 COMPOSED OF RX(74), RX(111)

RX(223) BZ + DP ==> EZ

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EZ
YIELD 62%

RX(74) RCT BZ 774217-21-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DN 774217-58-2
NTE chemoselective

RX(111) RCT DN 774217-58-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

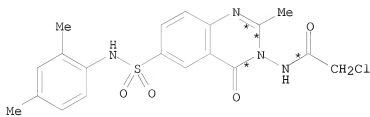
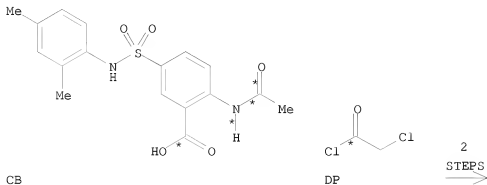
10/ 562,112

CON cooled

PRO EZ 774217-96-8

RX(224) OF 372 COMPOSED OF RX(75), RX(112)

RX(224) CB + DP ==> FA



FA
YIELD 70%

RX(75) RCT CB 774217-22-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DO 774217-59-3

NTE chemoselective

RX(112) RCT DO 774217-59-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

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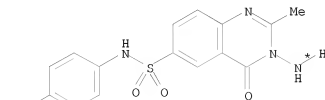
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO FA 774217-97-9

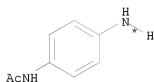
RX(249) OF 372 COMPOSED OF RX(100), RX(137)

RX(249) DC + DP + BA ==> FZ



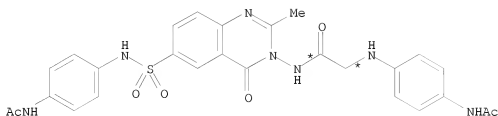
DC

DP



BA

2
STEPS
→



FZ

YIELD 53%

RX(100) RCT DC 774217-46-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

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CON cooled

PRO EO 774217-84-4

RX(137) RCT BA 122-80-5, EO 774217-84-4

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

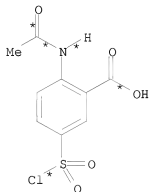
RGT D 7732-18-5 Water

CON cooled

PRO FZ 774218-18-7

RX(262) OF 372 COMPOSED OF RX(1), RX(39), RX(76)

RX(262) A + B + DP ==> DQ



A

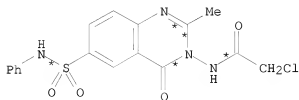


B



DP

3
STEPS
=>



DQ

YIELD 61%

RX(1) RCT A 181478-44-4, B 62-53-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO C 774216-86-3

RX(39) RCT C 774216-86-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CC 774217-23-1
NTE chemoselective

RX(76) RCT CC 774217-23-1, DP 79-04-9

STAGE(1)

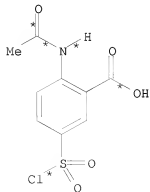
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

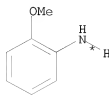
RGT D 7732-18-5 Water
CON cooled

PRO DQ 774217-60-6

RX(263) OF 372 COMPOSED OF RX(2), RX(40), RX(77)
RX(263) A + G + DP ==> DR



A

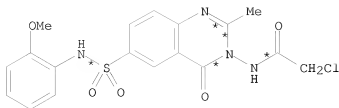


G



DP

3
STEPS
→



DR
YIELD 59%

RX(2) RCT A 181478-44-4, G 90-04-0

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO H 774216-87-4

RX(40) RCT H 774216-87-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CF 774217-24-2

NTE chemoselective

RX(77) RCT CF 774217-24-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

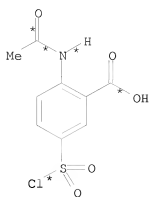
RGT D 7732-18-5 Water
CON cooled

PRO DR 774217-61-7

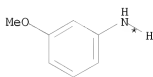
RX(264) OF 372 COMPOSED OF RX(3), RX(41), RX(78)

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RX(264) A + I + DP ==> DS



A

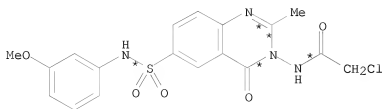


I



DP

3
STEPS
→



DS

YIELD 53%

RX(3) RCT A 181478-44-4, I 536-90-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO J 774216-88-5

RX(41) RCT J 774216-88-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

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CON cooled

PRO CG 774217-25-3
NTE chemoselective

RX(78) RCT CG 774217-25-3, DP 79-04-9

STAGE(1)

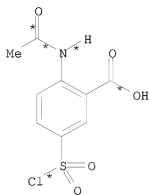
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

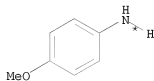
RGT D 7732-18-5 Water
CON cooled

PRO DS 774217-62-8

RX(265) OF 372 COMPOSED OF RX(4), RX(42), RX(79)
RX(265) A + K + DP ==> DT



A

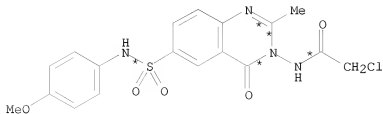


K



DP

3
STEPS
→



DT

YIELD 63%

RX(4) RCT A 181478-44-4, K 104-94-9

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO L 774216-89-6

RX(42) RCT L 774216-89-6

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CH 774217-26-4
NIE chemoselective

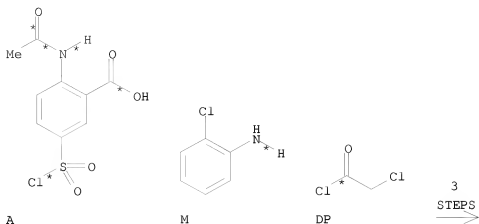
RX(79) RCT CH 774217-26-4, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DT 774217-63-9

RX(266) OF 372 COMPOSED OF RX(5), RX(43), RX(80)
RX(266) A + M + DP ==> DU



DU
YIELD 53%

RX(5) RCT A 181478-44-4, M 95-51-2

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO N 774216-90-9

RX(43) RCT N 774216-90-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

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PRO CI 774217-27-5
NTE chemoselective

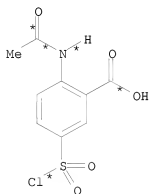
RX(80) RCT CI 774217-27-5, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

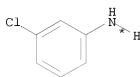
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DU 774217-64-0

RX(267) OF 372 COMPOSED OF RX(6), RX(44), RX(81)
RX(267) A + O + DP ==> DV



A

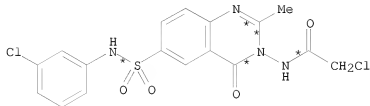


O



DP

3
STEPS
→



DV
YIELD 59%

RX(6) RCT A 181478-44-4, O 108-42-9

STAGE(1)
CAT 110-86-1 Pyridine

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SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO P 774216-91-0

RX(44) RCT P 774216-91-0

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CJ 774217-28-6
NTE chemoselective

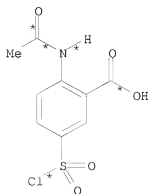
RX(81) RCT CJ 774217-28-6, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

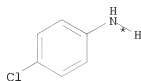
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DV 774217-65-1

RX(268) OF 372 COMPOSED OF RX(7), RX(45), RX(82)
RX(268) A + Q + DP ==> DW



A

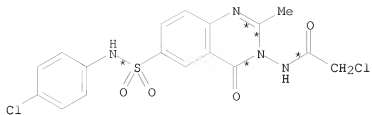


Q



DP

3
STEPS
→



DW
YIELD 58%

RX(7) RCT A 181478-44-4, Q 106-47-8

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO R 774216-92-1

RX(45) RCT R 774216-92-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CK 774217-29-7
NTE chemoselective

RX(82) RCT CK 774217-29-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

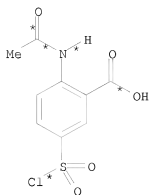
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

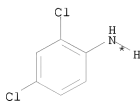
PRO DW 774217-66-2

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RX(269) OF 372 COMPOSED OF RX(8), RX(46), RX(83)
RX(269) A + S + DP ==> DX



A

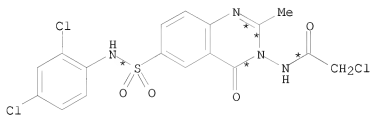


S



DP

3
STEPS
→



DX

YIELD 63%

RX(8) RCT A 181478-44-4, S 554-00-7

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO T 774216-93-2

RX(46) RCT T 774216-93-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

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RGT D 7732-18-5 Water
CON cooled

PRO CL 774217-30-0
NTE chemoselective

RX(83) RCT CL 774217-30-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

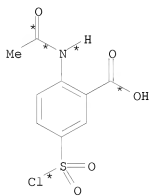
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

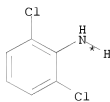
PRO DX 774217-67-3

RX(270) OF 372 COMPOSED OF RX(9), RX(47), RX(84)

RX(270) A + U + DP ==> DY



A

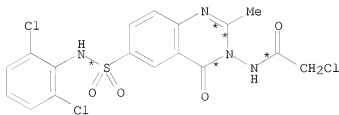


U



DP

3
STEPS
→



DY
YIELD 57%

RX(9) RCT A 181478-44-4, U 608-31-1


```
STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
    SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO V 774216-94-3

RX(47) RCT V 774216-94-3

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CM 774217-31-1
NTE chemoselective

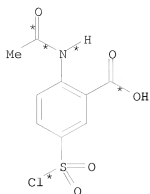
RX(84) RCT CM 774217-31-1, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
    SUBSTAGE(2) cooled

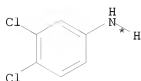
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DY 774217-68-4

RX(271) OF 372 COMPOSED OF RX(10), RX(48), RX(85)
RX(271) A + W + DP ==> DZ
```



A

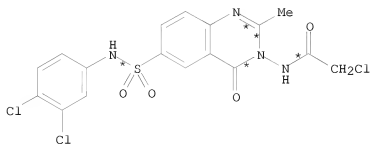


W



DP

3
STEPS
→



DZ
YIELD 57%

RX(10) RCT A 181478-44-4, W 95-76-1

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO X 774216-95-4

RX(48) RCT X 774216-95-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

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CON cooled

PRO CN 774217-32-2
NTE chemoselective

RX(85) RCT CN 774217-32-2, DP 79-04-9

STAGE(1)

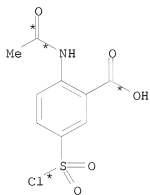
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

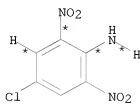
RGT D 7732-18-5 Water
CON cooled

PRO DZ 774217-69-5

RX(272) OF 372 COMPOSED OF RX(11), RX(49), RX(86)
RX(272) A + Y + DP ==> EA



A

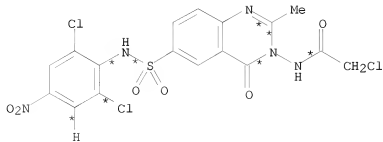


Y



DP

3
STEPS
→



EA
YIELD 62%

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RX(11) RCT A 181478-44-4, Y 5388-62-5

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO Z 218617-81-3

RX(49) RCT Z 218617-81-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CO 234096-58-3

NTE chemoselective

RX(86) RCT CO 234096-58-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

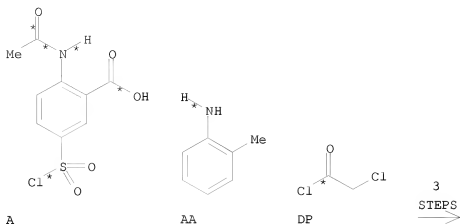
RGT D 7732-18-5 Water

CON cooled

PRO EA 774217-70-8

RX(273) OF 372 COMPOSED OF RX(12), RX(50), RX(87)

RX(273) A + AA + DP ==> EB



EB
YIELD 59%

RX(12) RCT A 181478-44-4, AA 95-53-4

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO AB 774216-96-5

RX(50) RCT AB 774216-96-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

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PRO CP 774217-33-3
NTE chemoselective

RX(87) RCT CP 774217-33-3, DP 79-04-9

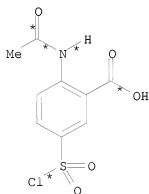
STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

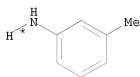
PRO EB 774217-71-9

RX(274) OF 372 COMPOSED OF RX(13), RX(51), RX(88)

RX(274) A + AC + DP ==> EC



A

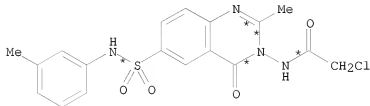


AC



DP

3
STEPS
→



EC
YIELD 64%

RX(13) RCT A 181478-44-4, AC 108-44-1

STAGE(1)
CAT 110-86-1 Pyridine

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SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AD 774216-97-6

RX(51) RCT AD 774216-97-6

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CQ 774217-34-4
NTE chemoselective

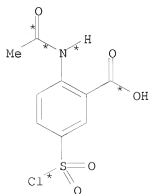
RX(88) RCT CQ 774217-34-4, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

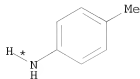
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EC 774217-72-0

RX(275) OF 372 COMPOSED OF RX(14), RX(52), RX(89)
RX(275) A + AE + DP ==> ED



A

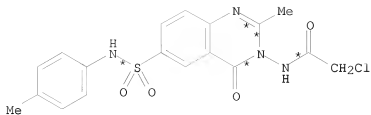


AE



DP

3
STEPS
→



ED
YIELD 63%

RX(14) RCT A 181478-44-4, AE 106-49-0

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO AF 774216-98-7

RX(52) RCT AF 774216-98-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CR 774217-35-5
NTE chemoselective

RX(89) RCT CR 774217-35-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

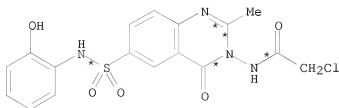
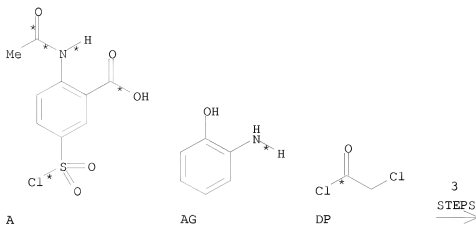
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO ED 774217-73-1

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RX(276) OF 372 COMPOSED OF RX(15), RX(53), RX(90)
RX(276) A + AG + DP ==> EE



EE
YIELD 58%

RX(15) RCT A 181478-44-4, AG 95-55-6

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AH 774216-99-8

RX(53) RCT AH 774216-99-8

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

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RGT D 7732-18-5 Water
CON cooled

PRO CS 774217-36-6
NTE chemoselective

RX(90) RCT CS 774217-36-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

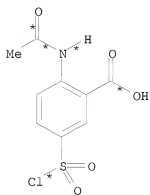
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

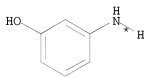
PRO EE 774217-74-2

RX(277) OF 372 COMPOSED OF RX(16), RX(54), RX(91)

RX(277) A + AI + DP ==> EF



A

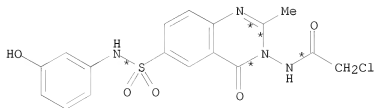


AI



DP

3
STEPS
→



EF
YIELD 59%

RX(16) RCT A 181478-44-4, AI 591-27-5

```
STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
    SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AJ 774217-00-4

RX(54) RCT AJ 774217-00-4

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CT 774217-37-7
NTE chemoselective

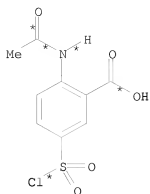
RX(91) RCT CT 774217-37-7, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
    SUBSTAGE(2) cooled

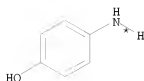
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EF 774217-75-3

RX(278) OF 372 COMPOSED OF RX(17), RX(55), RX(92)
RX(278) A + AK + DP ==> EG
```



A

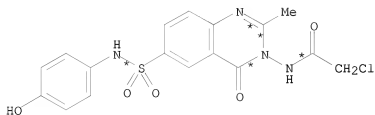


AK



DP

3
STEPS
→



EG

YIELD 63%

RX(17) RCT A 181478-44-4, AK 123-30-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AL 774217-01-5

RX(55) RCT AL 774217-01-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

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PRO CU 774217-38-8
NTE chemoselective

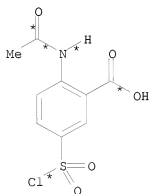
RX(92) RCT CU 774217-38-8, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

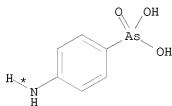
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EG 774217-76-4

RX(279) OF 372 COMPOSED OF RX(18), RX(56), RX(93)
RX(279) A + AM + DP ==> EH



A

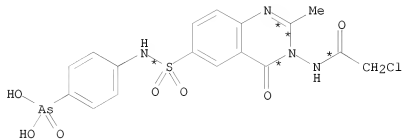


AM



DP

3
STEPS
=>



EH
YIELD 71%

RX(18) RCT A 181478-44-4, AM 98-50-0

```

      STAGE(1)
      CAT 110-86-1 Pyridine
      SOL 64-17-5 EtOH
      CON SUBSTAGE(1) 4 hours, 120 deg C
          SUBSTAGE(2) cooled

      STAGE(2)
      RGT D 7732-18-5 Water
      CON cooled

PRO   AN 774217-02-6

RX(56) RCT AN 774217-02-6

      STAGE(1)
      RGT CD 7803-57-8 N2H4-H2O
      SOL 67-56-1 MeOH
      CON 3 hours, reflux

      STAGE(2)
      RGT D 7732-18-5 Water
      CON cooled

PRO   CV 774217-39-9
NIE   chemoselective

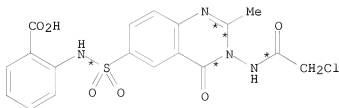
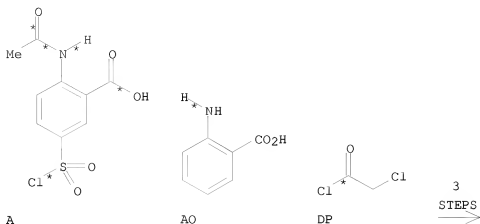
RX(93) RCT CV 774217-39-9, DP 79-04-9

      STAGE(1)
      RGT E 110-86-1 Pyridine
      SOL 64-17-5 EtOH
      CON SUBSTAGE(1) 4 hours, 120 deg C
          SUBSTAGE(2) cooled

      STAGE(2)
      RGT D 7732-18-5 Water
      CON cooled

PRO   EH 774217-77-5

RX(280) OF 372 COMPOSED OF RX(19), RX(57), RX(94)
RX(280) A + AO + DP ==> EI
```



EI
YIELD 75%

RX(19) RCT A 181478-44-4, AO 118-92-3

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO AP 774217-03-7

RX(57) RCT AP 774217-03-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

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PRO CW 774217-40-2
NTE chemoselective

RX(94) RCT CW 774217-40-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

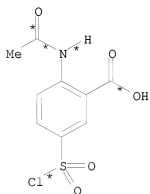
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

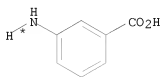
PRO EI 774217-78-6

RX(281) OF 372 COMPOSED OF RX(20), RX(58), RX(95)

RX(281) A + AQ + DP ==> EJ



A

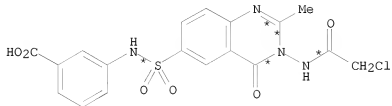


AQ



DP

3
STEPS
→



EJ

YIELD 70%

RX(20) RCT A 181478-44-4, AQ 99-05-8

STAGE(1)

CAT 110-86-1 Pyridine

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SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AR 774217-04-8

RX(58) RCT AR 774217-04-8

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CX 774217-41-3
NTE chemoselective

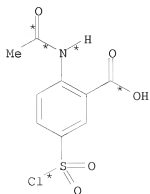
RX(95) RCT CX 774217-41-3, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

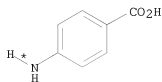
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EJ 774217-79-7

RX(282) OF 372 COMPOSED OF RX(21), RX(59), RX(96)
RX(282) A + AS + DP ==> EK



A

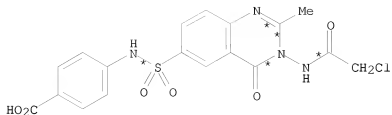


AS



DP

3
STEPS
→



EK
YIELD 68%

RX(21) RCT A 181478-44-4, AS 150-13-0

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO AT 774217-05-9

RX(59) RCT AT 774217-05-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CY 774217-42-4
NTE chemoselective

RX(96) RCT CY 774217-42-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

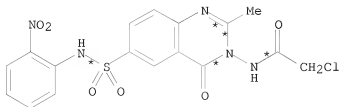
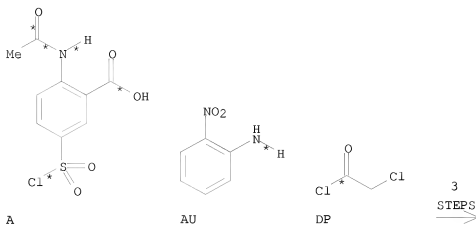
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EK 774217-80-0

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RX(283) OF 372 COMPOSED OF RX(22), RX(60), RX(97)
RX(283) A + AU + DP ==> EL



EL
YIELD 75%

RX(22) RCT A 181478-44-4, AU 88-74-4

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AV 774217-06-0

RX(60) RCT AV 774217-06-0

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

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RGT D 7732-18-5 Water
CON cooled

PRO CZ 774217-43-5
NTE chemoselective

RX(97) RCT CZ 774217-43-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

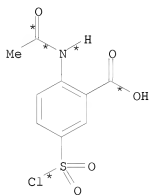
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

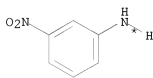
PRO EL 774217-81-1

RX(284) OF 372 COMPOSED OF RX(23), RX(61), RX(98)

RX(284) A + AW + DP ==> EM



A

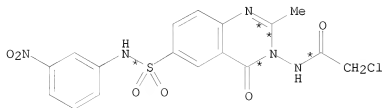


AW



DP

3
STEPS
→



EM
YIELD 78%

RX(23) RCT A 181478-44-4, AW 99-09-2

```
STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
    SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AX 774217-07-1

RX(61) RCT AX 774217-07-1

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DA 774217-44-6
NTE chemoselective

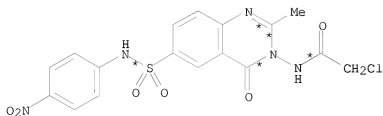
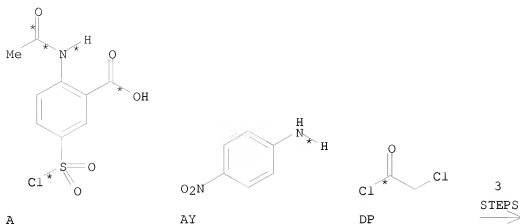
RX(98) RCT DA 774217-44-6, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
    SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EM 774217-82-2

RX(285) OF 372 COMPOSED OF RX(24), RX(62), RX(99)
RX(285) A + AY + DP ==> EN
```



EN
YIELD 71%

RX(24) RCT A 181478-44-4, AY 100-01-6

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO AZ 774217-08-2

RX(62) RCT AZ 774217-08-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

10/ 562,112

PRO DB 774217-45-7
NTE chemoselective

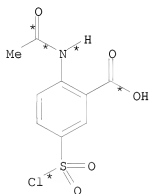
RX(99) RCT DB 774217-45-7, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

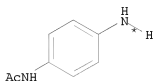
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EN 774217-83-3

RX(286) OF 372 COMPOSED OF RX(25), RX(63), RX(100)
RX(286) A + BA + DP ==> EO



A

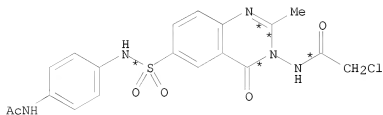


BA



DP

3
STEPS
→



EO
YIELD 53%

RX(25) RCT A 181478-44-4, BA 122-80-5

STAGE(1)
CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)
 RGT D 7732-18-5 Water
 CON cooled

PRO BB 774217-09-3

RX(63) RCT BB 774217-09-3

STAGE(1)
 RGT CD 7803-57-8 N2H4-H2O
 SOL 67-56-1 MeOH
 CON 3 hours, reflux

STAGE(2)
 RGT D 7732-18-5 Water
 CON cooled

PRO DC 774217-46-8
 NTE chemoselective

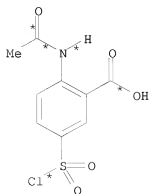
RX(100) RCT DC 774217-46-8, DP 79-04-9

STAGE(1)
 RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

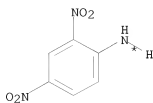
STAGE(2)
 RGT D 7732-18-5 Water
 CON cooled

PRO EO 774217-84-4

RX(287) OF 372 COMPOSED OF RX(26), RX(64), RX(101)
 RX(287) A + BC + DP ==> EP



A

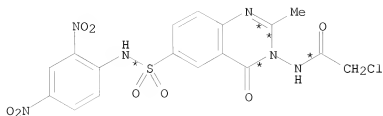


BC



DP

3
 STEPS



EP
YIELD 57%

RX(26) RCT A 181478-44-4, BC 97-02-9

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BD 774217-10-6

RX(64) RCT BD 774217-10-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DD 774217-47-9
NTE chemoselective

RX(101) RCT DD 774217-47-9, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

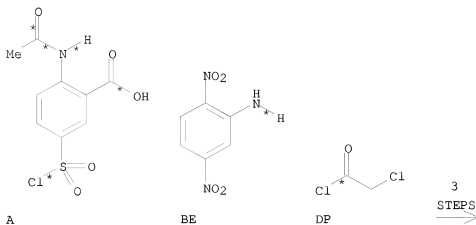
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EP 774217-85-5

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RX(288) OF 372 COMPOSED OF RX(27), RX(65), RX(102)
RX(288) A + BE + DP ==> EQ



EQ
YIELD 57%

RX(27) RCT A 181478-44-4, BE 619-18-1

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BF 774217-11-7

RX(65) RCT BF 774217-11-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

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STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DE 774217-48-0

NTE chemoselective

RX(102) RCT DE 774217-48-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

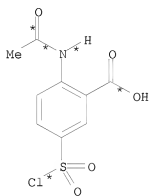
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

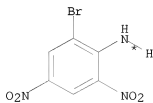
PRO EQ 774217-86-6

RX(289) OF 372 COMPOSED OF RX(28), RX(66), RX(103)

RX(289) A + BG + DP ==> ER



A

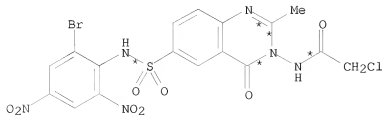


BG



DP

3
STEPS
→



ER

YIELD 54%

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RX(28) RCT A 181478-44-4, BG 1817-73-8

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BH 774217-12-8

RX(66) RCT BH 774217-12-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DF 774217-49-1

NTE chemoselective

RX(103) RCT DF 774217-49-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

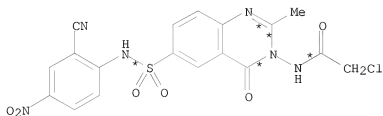
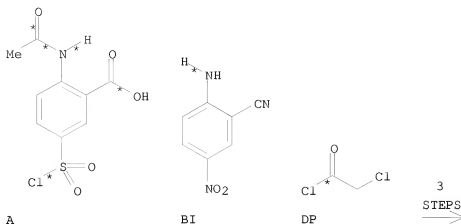
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO ER 774217-87-7

RX(290) OF 372 COMPOSED OF RX(29), RX(67), RX(104)

RX(290) A + BI + DP ==> ES



ES
YIELD 51%

RX(29) RCT A 181478-44-4, BI 17420-30-3

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BJ 774217-13-9

RX(67) RCT BJ 774217-13-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

10/ 562,112

PRO DG 774217-50-4
NTE chemoselective

RX(104) RCT DG 774217-50-4, DP 79-04-9

STAGE(1)

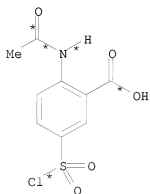
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

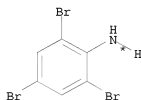
RGT D 7732-18-5 Water
CON cooled

PRO ES 774217-88-8

RX(291) OF 372 COMPOSED OF RX(30), RX(68), RX(105)
RX(291) A + BK + DP ==> ET



A

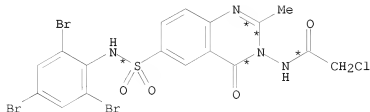


BK



DP

3
STEPS
→



ET
YIELD 58%

RX(30) RCT A 181478-44-4, BK 147-82-0

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)
 RGT D 7732-18-5 Water
 CON cooled

PRO BL 774217-14-0

RX(68) RCT BL 774217-14-0

STAGE(1)
 RGT CD 7803-57-8 N2H4-H2O
 SOL 67-56-1 MeOH
 CON 3 hours, reflux

STAGE(2)
 RGT D 7732-18-5 Water
 CON cooled

PRO DH 774217-51-5
 NTE chemoselective

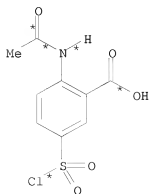
RX(105) RCT DH 774217-51-5, DP 79-04-9

STAGE(1)
 RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

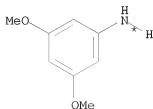
STAGE(2)
 RGT D 7732-18-5 Water
 CON cooled

PRO ET 774217-89-9

RX(292) OF 372 COMPOSED OF RX(31), RX(69), RX(106)
 RX(292) A + BM + DP ==> EU



A

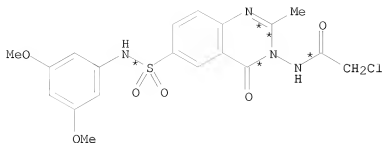


BM



DP

3
 STEPS
 →



EU

YIELD 63%

RX(31) RCT A 181478-44-4, BM 10272-07-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BN 774217-15-1

RX(69) RCT BN 774217-15-1

STAGE(1)

RGT CD 7803-57-8 N₂H₄-H₂O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DI 774217-52-6

NTE chemoselective

RX(106) RCT DI 774217-52-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

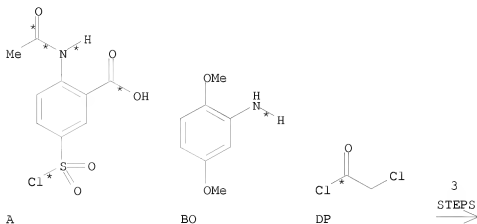
STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EU 774217-90-2

RX(293) OF 372 COMPOSED OF RX(32), RX(70), RX(107)
 RX(293) A + BO + DP ==> EV



EV
 YIELD 63%

RX(32) RCT A 181478-44-4, BO 102-56-7

STAGE(1)
 CAT 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)
 RGT D 7732-18-5 Water
 CON cooled

PRO BP 774217-16-2

RX(70) RCT BP 774217-16-2

STAGE(1)
 RGT CD 7803-57-8 N2H4-H2O

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SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DJ 774217-53-7
NTE chemoselective

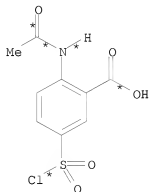
RX(107) RCT DJ 774217-53-7, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

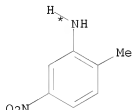
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EV 774217-91-3

RX(294) OF 372 COMPOSED OF RX(33), RX(71), RX(108)
RX(294) A + BQ + DP ==> EW



A

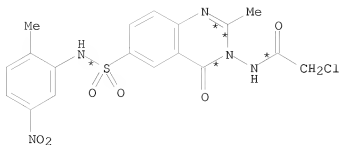


BQ



DP

3
STEPS
→



EW
YIELD 58%

RX(33) RCT A 181478-44-4, BQ 99-55-8

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BR 774217-17-3

RX(71) RCT BR 774217-17-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DK 774217-54-8

NTE chemoselective

RX(108) RCT DK 774217-54-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

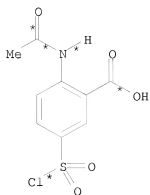
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

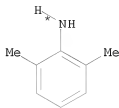
PRO EW 774217-92-4

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RX(295) OF 372 COMPOSED OF RX(35), RX(72), RX(109)
RX(295) A + BU + DP ==> EX



A

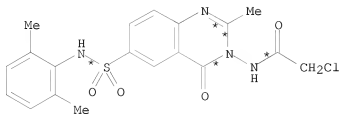


BU



DP

3
STEPS
→



EX

YIELD 56%

RX(35) RCT A 181478-44-4, BU 87-62-7

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BV 774217-19-5

RX(72) RCT BV 774217-19-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

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RGT D 7732-18-5 Water
CON cooled

PRO DL 774217-56-0
NTE chemoselective

RX(109) RCT DL 774217-56-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

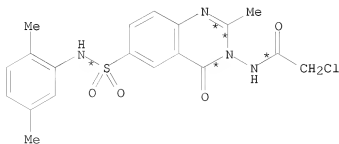
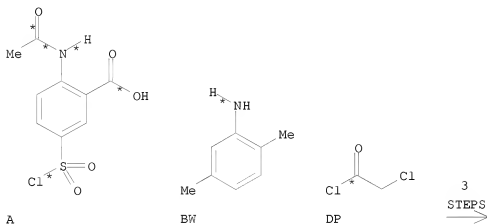
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EX 774217-94-6

RX(296) OF 372 COMPOSED OF RX(36), RX(73), RX(110)

RX(296) A + BW + DP ==> EY



EY
YIELD 59%

RX(36) RCT A 181478-44-4, BW 95-78-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BX 774217-20-8

RX(73) RCT BX 774217-20-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DM 774217-57-1

NTE chemoselective

RX(110) RCT DM 774217-57-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

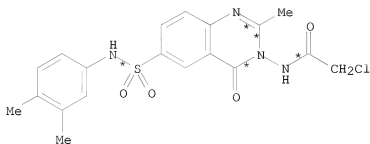
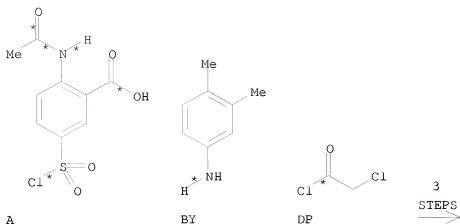
CON cooled

PRO EY 774217-95-7

RX(297) OF 372 COMPOSED OF RX(37), RX(74), RX(111)

RX(297) A + BY + DP ==> EZ

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EZ
YIELD 62%

RX(37) RCT A 181478-44-4, BY 95-64-7

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO BZ 774217-21-9

RX(74) RCT BZ 774217-21-9

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water

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CON cooled

PRO DN 774217-58-2
NTE chemoselective

RX(111) RCT DN 774217-58-2, DP 79-04-9

STAGE(1)

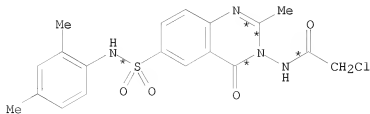
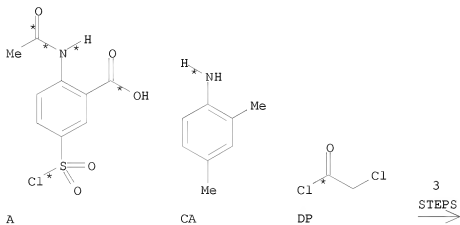
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EZ 774217-96-8

RX(298) OF 372 COMPOSED OF RX(38), RX(75), RX(112)
RX(298) A + CA + DP ==> FA



FA
YIELD 70%

RX(38) RCT A 181478-44-4, CA 95-68-1

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CB 774217-22-0

RX(75) RCT CB 774217-22-0

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DO 774217-59-3
NIE chemoselective

RX(112) RCT DO 774217-59-3, DP 79-04-9

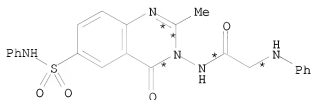
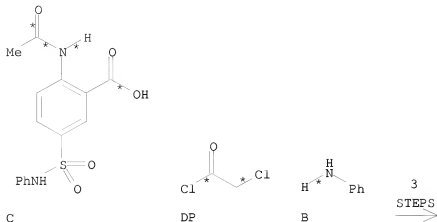
STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO FA 774217-97-9

RX(299) OF 372 COMPOSED OF RX(39), RX(76), RX(113)

RX(299) C + DP + B ==> FB



FB
YIELD 52%

RX(39) RCT C 774216-86-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CC 774217-23-1
NTE chemoselective

RX(76) RCT CC 774217-23-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

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PRO DQ 774217-60-6

RX(113) RCT B 62-53-3, DQ 774217-60-6

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

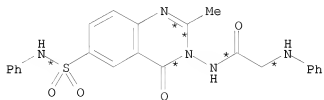
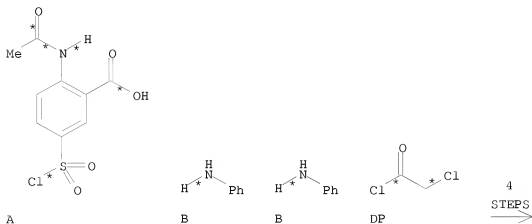
RGT D 7732-18-5 Water

CON cooled

PRO FB 774217-98-0

RX(300) OF 372 COMPOSED OF RX(1), RX(39), RX(76), RX(113)

RX(300) A + 2 B + DP ==> FB



FB
YIELD 52%

RX(1) RCT A 181478-44-4, B 62-53-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO C 774216-86-3

RX(39) RCT C 774216-86-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooledPRO CC 774217-23-1
NTE chemoselective

RX(76) RCT CC 774217-23-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DQ 774217-60-6

RX(113) RCT B 62-53-3, DQ 774217-60-6

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

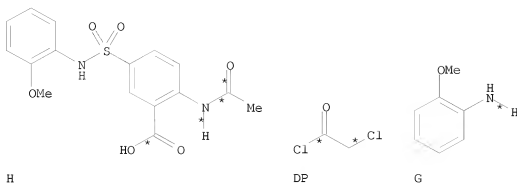
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

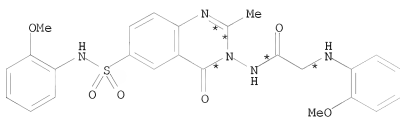
PRO FB 774217-98-0

RX(301) OF 372 COMPOSED OF RX(40), RX(77), RX(114)
RX(301) H + DP + G ==> FC

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3
STEPS
→



FC
YIELD 51%

RX(40) RCT H 774216-87-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CF 774217-24-2

NTE chemoselective

RX(77) RCT CF 774217-24-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

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RGT D 7732-18-5 Water
CON cooled

PRO DR 774217-61-7

RX(114) RCT G 90-04-0, DR 774217-61-7

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

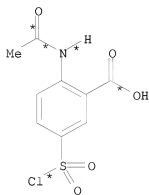
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

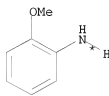
PRO FC 248259-39-4

RX(302) OF 372 COMPOSED OF RX(2), RX(40), RX(77), RX(114)

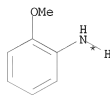
RX(302) A + 2 G + DP ==> FC



A



G

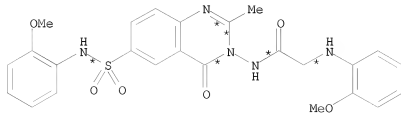


G



DP

4
STEPS
=>



FC
YIELD 51%

RX(2) RCT A 181478-44-4, G 90-04-0

```

      STAGE(1)
      CAT 110-86-1 Pyridine
      SOL 64-17-5 EtOH
      CON SUBSTAGE(1) 4 hours, 120 deg C
          SUBSTAGE(2) cooled

      STAGE(2)
      RGT D 7732-18-5 Water
      CON cooled

PRO   H 774216-87-4

RX(40) RCT H 774216-87-4

      STAGE(1)
      RGT CD 7803-57-8 N2H4-H2O
      SOL 67-56-1 MeOH
      CON 3 hours, reflux

      STAGE(2)
      RGT D 7732-18-5 Water
      CON cooled

PRO   CF 774217-24-2
NIE   chemoselective

RX(77) RCT CF 774217-24-2, DP 79-04-9

      STAGE(1)
      RGT E 110-86-1 Pyridine
      SOL 64-17-5 EtOH
      CON SUBSTAGE(1) 4 hours, 120 deg C
          SUBSTAGE(2) cooled

      STAGE(2)
      RGT D 7732-18-5 Water
      CON cooled

PRO   DR 774217-61-7

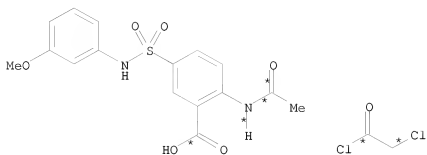
RX(114) RCT G 90-04-0, DR 774217-61-7

      STAGE(1)
      RGT E 110-86-1 Pyridine
      SOL 64-17-5 EtOH
      CON SUBSTAGE(1) 4 hours, 120 deg C
          SUBSTAGE(2) cooled

      STAGE(2)
      RGT D 7732-18-5 Water
      CON cooled

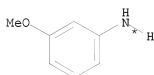
PRO   FC 248259-39-4

RX(303) OF 372 COMPOSED OF RX(41), RX(78), RX(115)
RX(303) J + DP + I ==> FD
```



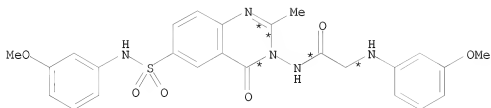
J

DP



I

3
STEPS
→



FD

YIELD 54%

RX(41) RCT J 774216-88-5

STAGE(1)

RGT CD 7803-57-8 N₂H₄-H₂O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CG 774217-25-3

NTE chemoselective

RX(78) RCT CG 774217-25-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

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SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DS 774217-62-8

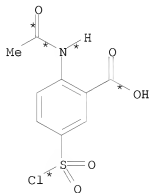
RX(115) RCT I 536-90-3, DS 774217-62-8

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

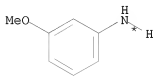
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO FD 774217-99-1

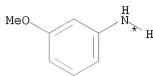
RX(304) OF 372 COMPOSED OF RX(3), RX(41), RX(78), RX(115)
RX(304) A + 2 I + DP ==> FD



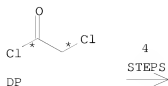
A



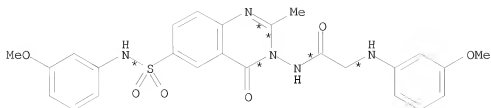
I



I



4
STEPS
→



FD
YIELD 54%

RX(3) RCT A 181478-44-4, I 536-90-3

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO J 774216-88-5

RX(41) RCT J 774216-88-5

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CG 774217-25-3
NTE chemoselective

RX(78) RCT CG 774217-25-3, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DS 774217-62-8

RX(115) RCT I 536-90-3, DS 774217-62-8

STAGE(1)

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RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

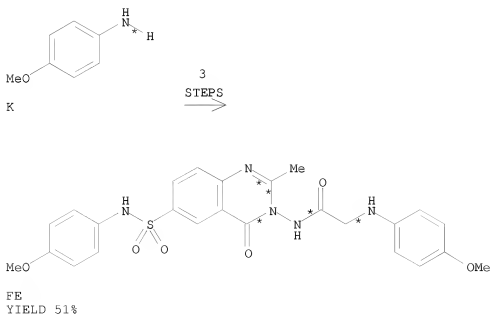
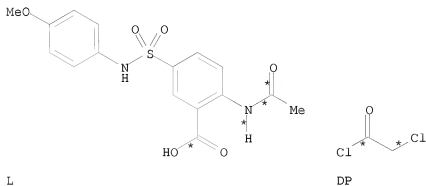
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO FD 774217-99-1

RX(305) OF 372 COMPOSED OF RX(42), RX(79), RX(116)

RX(305) L + DP + K ==> FE



RX(42) RCT L 774216-89-6

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CH 774217-26-4
NTE chemoselective

RX(79) RCT CH 774217-26-4, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DT 774217-63-9

RX(116) RCT K 104-94-9, DT 774217-63-9

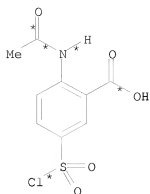
STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

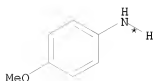
PRO FE 248259-41-8

RX(306) OF 372 COMPOSED OF RX(4), RX(42), RX(79), RX(116)

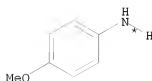
RX(306) A + 2 K + DP ==> FE



A



K

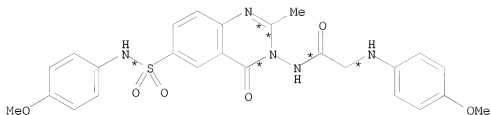


K



DP

4
STEPS
→



FE
YIELD 51%

RX(4) RCT A 181478-44-4, K 104-94-9

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO L 774216-89-6

RX(42) RCT L 774216-89-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
 SOL 67-56-1 MeOH
 CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO CH 774217-26-4
 NTE chemoselective

RX(79) RCT CH 774217-26-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO DT 774217-63-9

RX(116) RCT K 104-94-9, DT 774217-63-9

STAGE(1)

RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

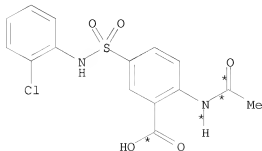
STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO FE 248259-41-8

RX(307) OF 372 COMPOSED OF RX(43), RX(80), RX(117)

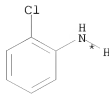
RX(307) N + DP + M ==> FF



N



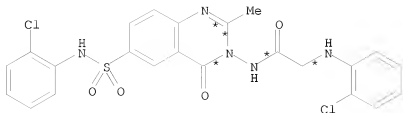
DP



M

10/ 562,112

3
STEPS
→



FF
YIELD 58%

RX(43) RCT N 774216-90-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CI 774217-27-5
NIE chemoselective

RX(80) RCT CI 774217-27-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DU 774217-64-0

RX(117) RCT M 95-51-2, DU 774217-64-0

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

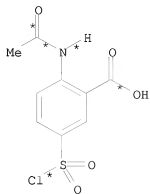
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

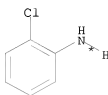
PRO FF 248259-42-9

RX(308) OF 372 COMPOSED OF RX(5), RX(43), RX(80), RX(117)

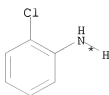
RX(308) A + 2 M + DP ==> FF



A



M

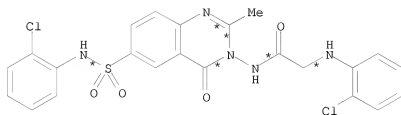


M



DP

4
STEPS
=>



FF
YIELD 58%

RX(5) RCT A 181478-44-4, M 95-51-2

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO N 774216-90-9

RX(43) RCT N 774216-90-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

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SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CI 774217-27-5
NTE chemoselective

RX(80) RCT CI 774217-27-5, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DU 774217-64-0

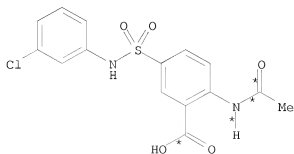
RX(117) RCT M 95-51-2, DU 774217-64-0

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO FF 248259-42-9

RX(309) OF 372 COMPOSED OF RX(44), RX(81), RX(118)
RX(309) P + DP + O ==> FG

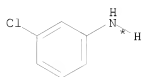


P



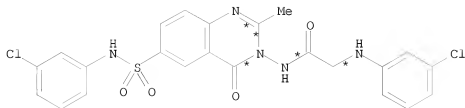
DP

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O

3
STEPS
→



FG

YIELD 58%

RX(44) RCT P 774216-91-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CJ 774217-28-6

NTE chemoselective

RX(81) RCT CJ 774217-28-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DV 774217-65-1

RX(118) RCT O 108-42-9, DV 774217-65-1

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

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STAGE(2)

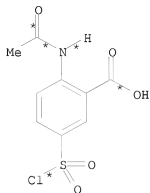
RGT D 7732-18-5 Water

CON cooled

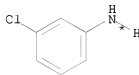
PRO FG 774218-00-7

RX(310) OF 372 COMPOSED OF RX(6), RX(44), RX(81), RX(118)

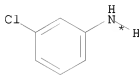
RX(310) A + 2 O + DP ==> FG



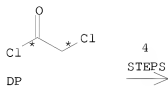
A



O

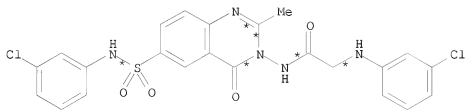


O



DP

4
STEPS
→



FG

YIELD 58%

RX(6) RCT A 181478-44-4, O 108-42-9

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO P 774216-91-0

RX(44) RCT P 774216-91-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CJ 774217-28-6

NTE chemoselective

RX(81) RCT CJ 774217-28-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DV 774217-65-1

RX(118) RCT O 108-42-9, DV 774217-65-1

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

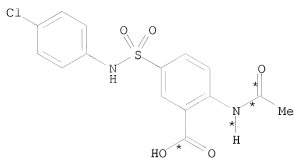
RGT D 7732-18-5 Water
CON cooled

PRO FG 774218-00-7

RX(311) OF 372 COMPOSED OF RX(45), RX(82), RX(119)

RX(311) R + DP + Q ==> FH

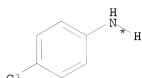
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R

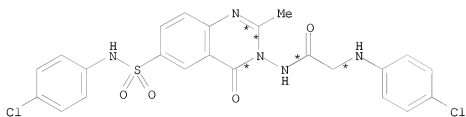


DP



Q

3
STEPS
→



FH

YIELD 62%

RX(45) RCT R 774216-92-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CK 774217-29-7

NTE chemoselective

RX(82) RCT CK 774217-29-7, DP 79-04-9

STAGE(1)

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RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DW 774217-66-2

RX(119) RCT Q 106-47-8, DW 774217-66-2

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

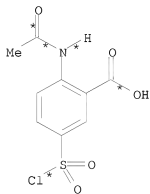
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

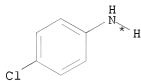
PRO FH 248259-43-0

RX(312) OF 372 COMPOSED OF RX(7), RX(45), RX(82), RX(119)

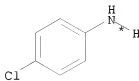
RX(312) A + 2 Q + DP ==> FH



A



Q

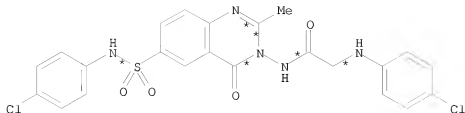


Q



DP

4
STEPS
→



FH
YIELD 62%

RX(7) RCT A 181478-44-4, Q 106-47-8

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO R 774216-92-1

RX(45) RCT R 774216-92-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CK 774217-29-7
NTE chemoselective

RX(82) RCT CK 774217-29-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DW 774217-66-2

RX(119) RCT Q 106-47-8, DW 774217-66-2

STAGE(1)

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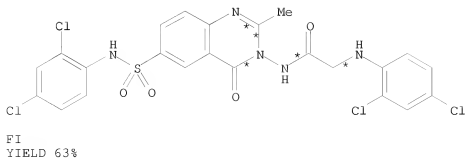
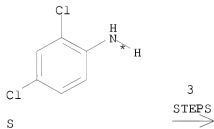
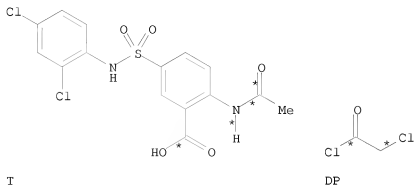
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO FH 248259-43-0

RX(313) OF 372 COMPOSED OF RX(46), RX(83), RX(120)
RX(313) T + DP + S ==> FI



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RX(46) RCT T 774216-93-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CL 774217-30-0

NTE chemoselective

RX(83) RCT CL 774217-30-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DX 774217-67-3

RX(120) RCT S 554-00-7, DX 774217-67-3

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

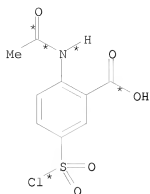
RGT D 7732-18-5 Water

CON cooled

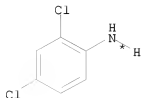
PRO FI 774218-01-8

RX(314) OF 372 COMPOSED OF RX(8), RX(46), RX(83), RX(120)

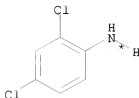
RX(314) A + 2 S + DP ==> FI



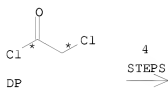
A



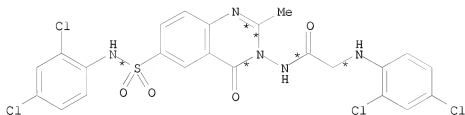
S



S



4
STEPS
→



FI
YIELD 63%

RX(8) RCT A 181478-44-4, S 554-00-7

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO T 774216-93-2

RX(46) RCT T 774216-93-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CL 774217-30-0

NTE chemoselective

RX(83) RCT CL 774217-30-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DX 774217-67-3

RX(120) RCT S 554-00-7, DX 774217-67-3

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

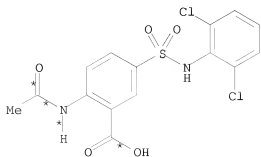
RGT D 7732-18-5 Water

CON cooled

PRO FI 774218-01-8

RX(315) OF 372 COMPOSED OF RX(47), RX(84), RX(121)

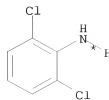
RX(315) V + DP + U ==> FJ



V



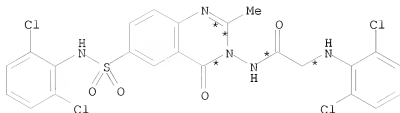
DP



U

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3
STEPS
→



FJ
YIELD 61%

RX(47) RCT V 774216-94-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CM 774217-31-1
NIE chemoselective

RX(84) RCT CM 774217-31-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DY 774217-68-4

RX(121) RCT U 608-31-1, DY 774217-68-4

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

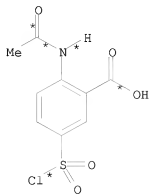
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

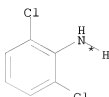
PRO FJ 774218-02-9

RX(316) OF 372 COMPOSED OF RX(9), RX(47), RX(84), RX(121)

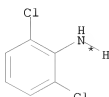
RX(316) A + 2 U + DP ==> FJ



A



U

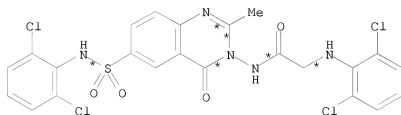


U



DP

4
STEPS
=>



FJ

YIELD 61%

RX(9) RCT A 181478-44-4, U 608-31-1

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO V 774216-94-3

RX(47) RCT V 774216-94-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

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SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CM 774217-31-1
NTE chemoselective

RX(84) RCT CM 774217-31-1, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DY 774217-68-4

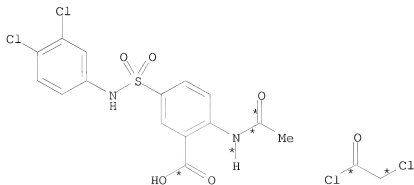
RX(121) RCT U 608-31-1, DY 774217-68-4

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO FJ 774218-02-9

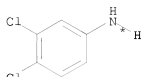
RX(317) OF 372 COMPOSED OF RX(48), RX(85), RX(122)
RX(317) X + DP + W ==> FK



X

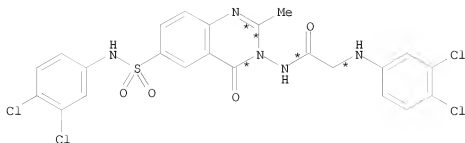
DP

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W

3
STEPS
→



FK

YIELD 64%

RX(48) RCT X 774216-95-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CN 774217-32-2

NIE chemoselective

RX(85) RCT CN 774217-32-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DZ 774217-69-5

RX(122) RCT W 95-76-1, DZ 774217-69-5

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STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

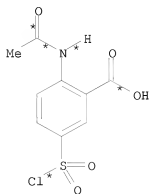
RGT D 7732-18-5 Water

CON cooled

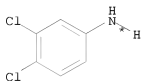
PRO FK 774218-03-0

RX(318) OF 372 COMPOSED OF RX(10), RX(48), RX(85), RX(122)

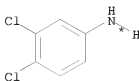
RX(318) A + 2 W + DP ==> FK



A



W

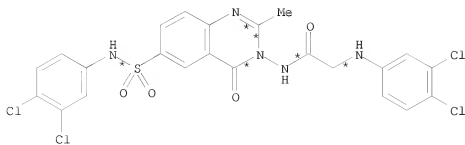


W



DP

4
STEPS
→



FK

YIELD 64%

RX(10) RCT A 181478-44-4, W 95-76-1

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO X 774216-95-4

RX(48) RCT X 774216-95-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CN 774217-32-2

NTE chemoselective

RX(85) RCT CN 774217-32-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DZ 774217-69-5

RX(122) RCT W 95-76-1, DZ 774217-69-5

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

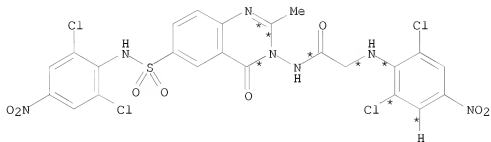
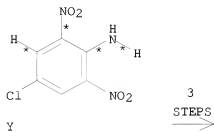
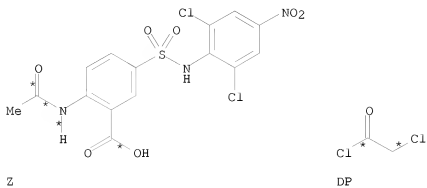
RGT D 7732-18-5 Water
CON cooled

PRO FK 774218-03-0

RX(319) OF 372 COMPOSED OF RX(49), RX(86), RX(123)

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RX(319) Z + DP + Y ==> FL



FL
YIELD 67%

RX(49) RCT Z 218617-81-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

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PRO CO 234096-58-3
NTE chemoselective

RX(86) RCT CO 234096-58-3, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EA 774217-70-8

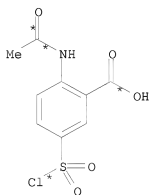
RX(123) RCT Y 5388-62-5, EA 774217-70-8

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

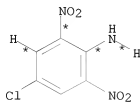
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO FL 774218-04-1

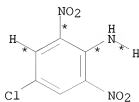
RX(320) OF 372 COMPOSED OF RX(11), RX(49), RX(86), RX(123)
RX(320) A + 2 Y + DP ==> FL



A

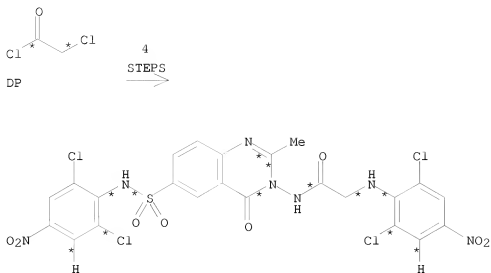


Y



Y

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RX(11) RCT A 181478-44-4, Y 5388-62-5

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO Z 218617-81-3

RX(49) RCT Z 218617-81-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CO 234096-58-3

NTE chemoselective

RX(86) RCT CO 234096-58-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

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SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EA 774217-70-8

RX(123) RCT Y 5388-62-5, EA 774217-70-8

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

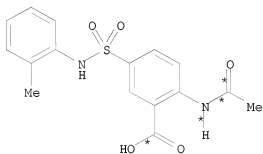
RGT D 7732-18-5 Water

CON cooled

PRO FL 774218-04-1

RX(321) OF 372 COMPOSED OF RX(50), RX(87), RX(124)

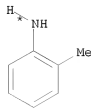
RX(321) AB + DP + AA ==> FM



AB

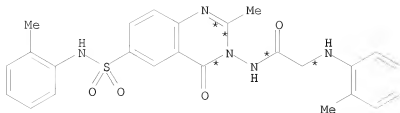


DP



AA

3
STEPS
→



FM

YIELD 54%

RX(50) RCT AB 774216-96-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
 SOL 67-56-1 MeOH
 CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO CP 774217-33-3

NTE chemoselective

RX(87) RCT CP 774217-33-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO EB 774217-71-9

RX(124) RCT AA 95-53-4, EB 774217-71-9

STAGE(1)

RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

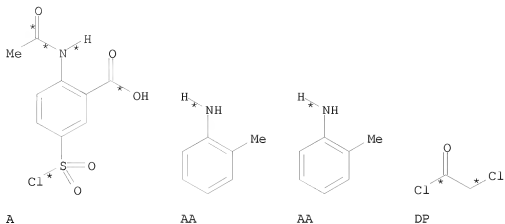
STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

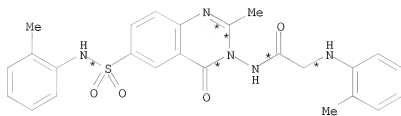
PRO FM 774218-05-2

RX(322) OF 372 COMPOSED OF RX(12), RX(50), RX(87), RX(124)

RX(322) A + 2 AA + DP ==> FM



4
STEPS
→



FM
YIELD 54%

RX(12) RCT A 181478-44-4, AA 95-53-4

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO AB 774216-96-5

RX(50) RCT AB 774216-96-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

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PRO CP 774217-33-3
NTE chemoselective

RX(87) RCT CP 774217-33-3, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EB 774217-71-9

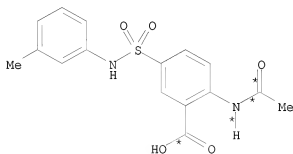
RX(124) RCT AA 95-53-4, EB 774217-71-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO FM 774218-05-2

RX(323) OF 372 COMPOSED OF RX(51), RX(88), RX(125)
RX(323) AD + DP + AC ==> FN

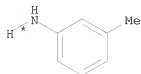


AD



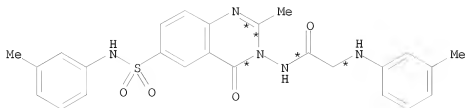
DP

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AC

3
STEPS
→



FN

YIELD 55%

RX(51) RCT AD 774216-97-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CQ 774217-34-4

NTE chemoselective

RX(88) RCT CQ 774217-34-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EC 774217-72-0

RX(125) RCT AC 108-44-1, EC 774217-72-0

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

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STAGE(2)

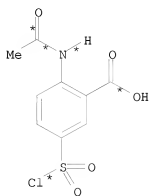
RGT D 7732-18-5 Water

CON cooled

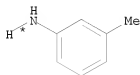
PRO FN 774218-06-3

RX(324) OF 372 COMPOSED OF RX(13), RX(51), RX(88), RX(125)

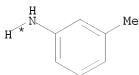
RX(324) A + 2 AC + DP ==> FN



A



AC

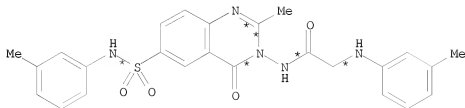


AC



DP

4
STEPS
→



FN

YIELD 55%

RX(13) RCT A 181478-44-4, AC 108-44-1

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AD 774216-97-6

RX(51) RCT AD 774216-97-6

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CQ 774217-34-4
NTE chemoselective

RX(88) RCT CQ 774217-34-4, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EC 774217-72-0

RX(125) RCT AC 108-44-1, EC 774217-72-0

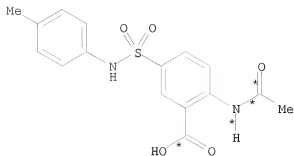
STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO FN 774218-06-3

RX(325) OF 372 COMPOSED OF RX(52), RX(89), RX(126)
RX(325) AF + DP + AE ==> FO

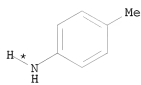
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AF

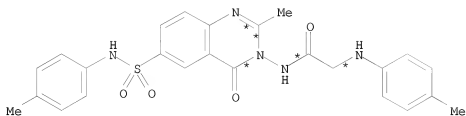


DP



AE

3
STEPS
→



FO

YIELD 52%

RX(52) RCT AF 774216-98-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CR 774217-35-5

NTE chemoselective

RX(89) RCT CR 774217-35-5, DP 79-04-9

STAGE(1)

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RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO ED 774217-73-1

RX(126) RCT AE 106-49-0, ED 774217-73-1

STAGE(1)

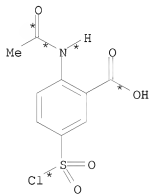
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

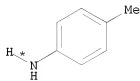
RGT D 7732-18-5 Water
CON cooled

PRO FO 774218-07-4

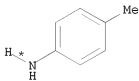
RX(326) OF 372 COMPOSED OF RX(14), RX(52), RX(89), RX(126)
RX(326) A + 2 AE + DP ==> FO



A



AE

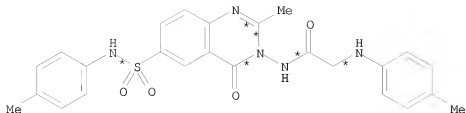


AE



DP

4
STEPS
→



FO
YIELD 52%

RX(14) RCT A 181478-44-4, AE 106-49-0

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AF 774216-98-7

RX(52) RCT AF 774216-98-7

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CR 774217-35-5
NTE chemoselective

RX(89) RCT CR 774217-35-5, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO ED 774217-73-1

RX(126) RCT AE 106-49-0, ED 774217-73-1

STAGE(1)

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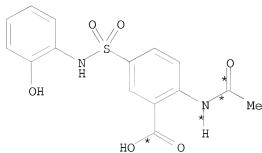
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO FO 774218-07-4

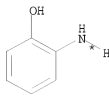
RX(327) OF 372 COMPOSED OF RX(53), RX(90), RX(127)
RX(327) AH + DP + AG ==> FP



AH

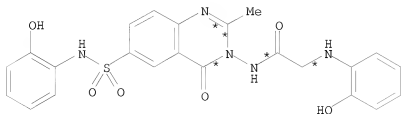


DP



AG

3
STEPS
→



FP
YIELD 56%

RX(53) RCT AH 774216-99-8

STAGE(1)

RGT CD 7803-57-8 N₂H₄-H₂O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

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RGT D 7732-18-5 Water
CON cooled

PRO CS 774217-36-6
NTE chemoselective

RX(90) RCT CS 774217-36-6, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EE 774217-74-2

RX(127) RCT AG 95-55-6, EE 774217-74-2

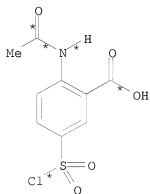
STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

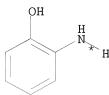
PRO FP 774218-08-5

RX(328) OF 372 COMPOSED OF RX(15), RX(53), RX(90), RX(127)

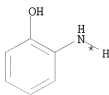
RX(328) A + 2 AG + DP ==> FP



A



AG

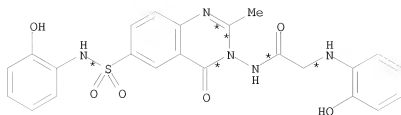


AG



DP

4
STEPS
→



FP
YIELD 56%

RX(15) RCT A 181478-44-4, AG 95-55-6

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO AH 774216-99-8

RX(53) RCT AH 774216-99-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CS 774217-36-6
NTE chemoselective

RX(90) RCT CS 774217-36-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EE 774217-74-2

RX(127) RCT AG 95-55-6, EE 774217-74-2

STAGE(1)

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RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

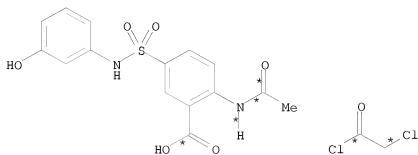
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO FP 774218-08-5

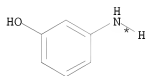
RX(329) OF 372 COMPOSED OF RX(54), RX(91), RX(128)

RX(329) AJ + DP + AI ==> FQ



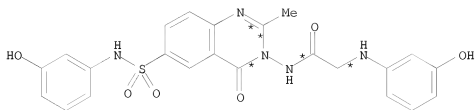
AJ

DP



AI

3
STEPS
→



FQ

YIELD 57%

RX(54) RCT AJ 774217-00-4

STAGE(1)

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RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CT 774217-37-7
NTE chemoselective

RX(91) RCT CT 774217-37-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EF 774217-75-3

RX(128) RCT AI 591-27-5, EF 774217-75-3

STAGE(1)

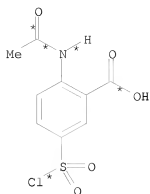
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

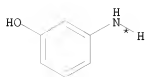
RGT D 7732-18-5 Water
CON cooled

PRO FQ 774218-09-6

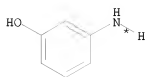
RX(330) OF 372 COMPOSED OF RX(16), RX(54), RX(91), RX(128)
RX(330) A + 2 AI + DP ==> FQ



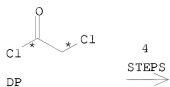
A



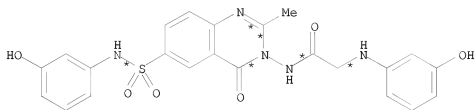
AI



AI



4
STEPS
→



FQ
YIELD 57%

RX(16) RCT A 181478-44-4, AI 591-27-5

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AJ 774217-00-4

RX(54) RCT AJ 774217-00-4

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
 SOL 67-56-1 MeOH
 CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO CT 774217-37-7
 NTE chemoselective

RX(91) RCT CT 774217-37-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO EF 774217-75-3

RX(128) RCT AI 591-27-5, EF 774217-75-3

STAGE(1)

RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

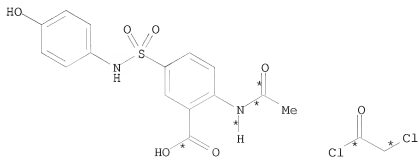
STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO FQ 774218-09-6

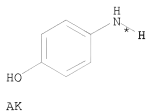
RX(331) OF 372 COMPOSED OF RX(55), RX(92), RX(129)

RX(331) AL + DP + AK ==> FR

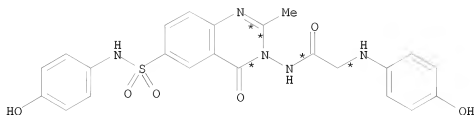


AL

DP



3
STEPS
→



FR
YIELD 52%

RX(55) RCT AL 774217-01-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CU 774217-38-8
NTE chemoselective

RX(92) RCT CU 774217-38-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EG 774217-76-4

RX(129) RCT AK 123-30-8, EG 774217-76-4

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

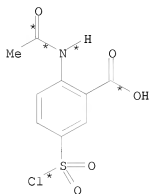
RGT D 7732-18-5 Water

CON cooled

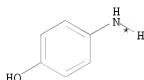
PRO FR 774218-10-9

RX(332) OF 372 COMPOSED OF RX(17), RX(55), RX(92), RX(129)

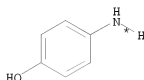
RX(332) A + 2 AK + DP ==> FR



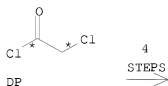
A



AK

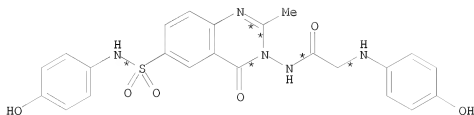


AK



DP

4
STEPS
→



FR

YIELD 52%

RX(17) RCT A 181478-44-4, AK 123-30-8

STAGE(1)

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CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AL 774217-01-5

RX(55) RCT AL 774217-01-5

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CU 774217-38-8
NTE chemoselective

RX(92) RCT CU 774217-38-8, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EG 774217-76-4

RX(129) RCT AK 123-30-8, EG 774217-76-4

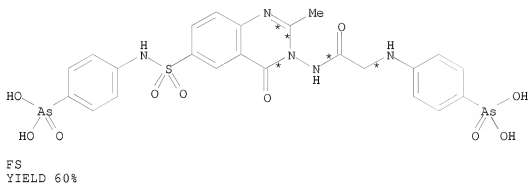
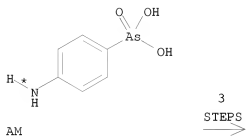
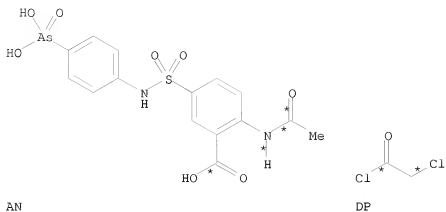
STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO FR 774218-10-9

RX(333) OF 372 COMPOSED OF RX(56), RX(93), RX(130)
RX(333) AN + DP + AM ==> FS

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RX(56) RCT AN 774217-02-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

10/ 562,112

PRO CV 774217-39-9
NTE chemoselective

RX(93) RCT CV 774217-39-9, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EH 774217-77-5

RX(130) RCT AM 98-50-0, EH 774217-77-5

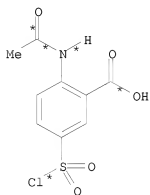
STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

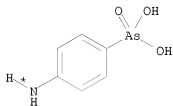
PRO FS 774218-11-0

RX(334) OF 372 COMPOSED OF RX(18), RX(56), RX(93), RX(130)

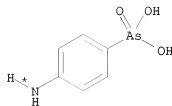
RX(334) A + 2 AM + DP ==> FS



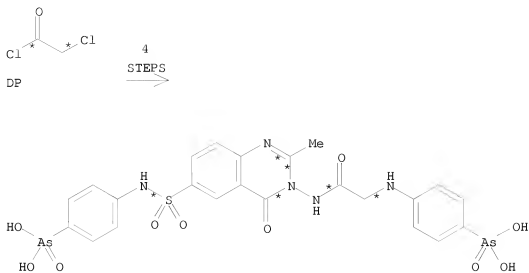
A



AM



AM



FS
YIELD 60%

RX(18) RCT A 181478-44-4, AM 98-50-0

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO AN 774217-02-6

RX(56) RCT AN 774217-02-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CV 774217-39-9

NTE chemoselective

RX(93) RCT CV 774217-39-9, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C

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SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EH 774217-77-5

RX(130) RCT AM 98-50-0, EH 774217-77-5

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

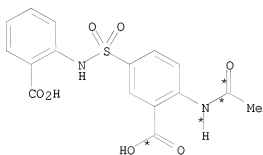
RGT D 7732-18-5 Water

CON cooled

PRO FS 774218-11-0

RX(335) OF 372 COMPOSED OF RX(57), RX(94), RX(131)

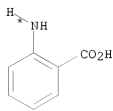
RX(335) AP + DP + AO ==> FT



AP

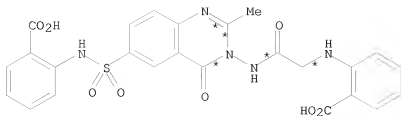


DP



AO

3
STEPS
→



FT
YIELD 63%

RX(57) RCT AP 774217-03-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO CW 774217-40-2
NTE chemoselective

RX(94) RCT CW 774217-40-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EI 774217-78-6

RX(131) RCT AO 118-92-3, EI 774217-78-6

STAGE(1)

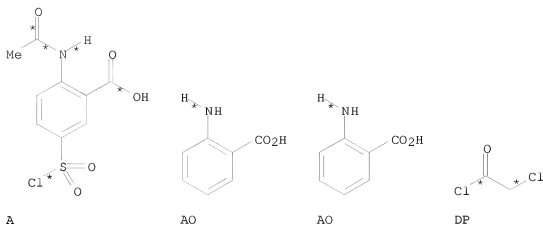
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

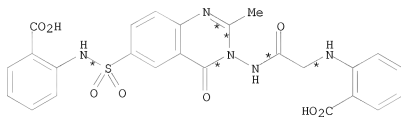
RGT D 7732-18-5 Water
CON cooled

PRO FT 774218-12-1

RX(336) OF 372 COMPOSED OF RX(19), RX(57), RX(94), RX(131)
RX(336) A + 2 AO + DP ==> FT



4
STEPS
→



FT
YIELD 63%

RX(19) RCT A 181478-44-4, AO 118-92-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AP 774217-03-7

RX(57) RCT AP 774217-03-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

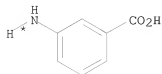
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

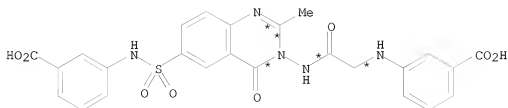
CON cooled

10/ 562,112



AQ

3
STEPS
→



FU

YIELD 61%

RX(58) RCT AR 774217-04-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CX 774217-41-3

NTE chemoselective

RX(95) RCT CX 774217-41-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EJ 774217-79-7

RX(132) RCT AQ 99-05-8, EJ 774217-79-7

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

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STAGE(2)

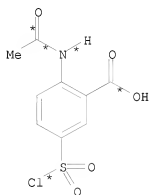
RGT D 7732-18-5 Water

CON cooled

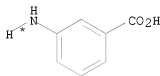
PRO FU 774218-13-2

RX(338) OF 372 COMPOSED OF RX(20), RX(58), RX(95), RX(132)

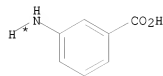
RX(338) A + 2 AQ + DP ==> FU



A



AQ

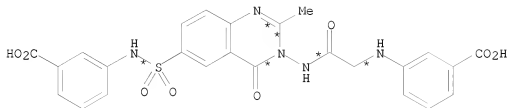


AQ



DP

4
STEPS
→



FU

YIELD 61%

RX(20) RCT A 181478-44-4, AQ 99-05-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AR 774217-04-8

RX(58) RCT AR 774217-04-8

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CX 774217-41-3
NTE chemoselective

RX(95) RCT CX 774217-41-3, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EJ 774217-79-7

RX(132) RCT AQ 99-05-8, EJ 774217-79-7

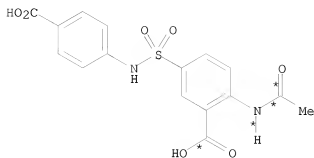
STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO FU 774218-13-2

RX(339) OF 372 COMPOSED OF RX(59), RX(96), RX(133)
RX(339) AT + DP + AS ==> FV

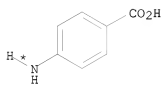
10/ 562,112



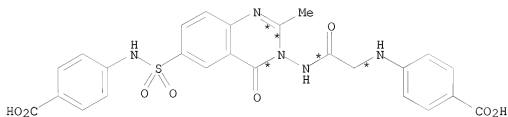
AT



DP



AS



FV

YIELD 63%

RX(59) RCT AT 774217-05-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CY 774217-42-4

NTE chemoselective

RX(96) RCT CY 774217-42-4, DP 79-04-9

STAGE(1)

10/ 562,112

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EK 774217-80-0

RX(133) RCT AS 150-13-0, EK 774217-80-0

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

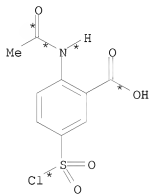
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

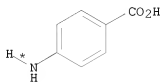
PRO FV 774218-14-3

RX(340) OF 372 COMPOSED OF RX(21), RX(59), RX(96), RX(133)

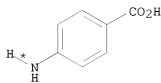
RX(340) A + 2 AS + DP ==> FV



A



AS

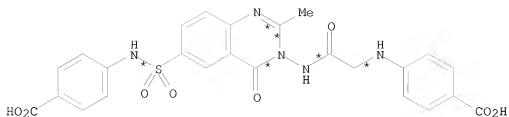


AS



DP

4
STEPS
→



FV

YIELD 63%

RX(21) RCT A 181478-44-4, AS 150-13-0

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AT 774217-05-9

RX(59) RCT AT 774217-05-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO CY 774217-42-4

NTE chemoselective

RX(96) RCT CY 774217-42-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EK 774217-80-0

RX(133) RCT AS 150-13-0, EK 774217-80-0

STAGE(1)

10/ 562,112

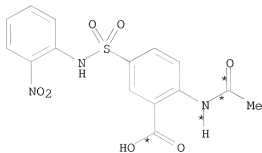
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO FV 774218-14-3

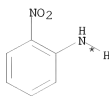
RX(341) OF 372 COMPOSED OF RX(60), RX(97), RX(134)
RX(341) AV + DP + AU ==> FW



AV

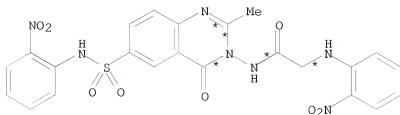


DP



AU

3
STEPS
→



FW
YIELD 65%

RX(60) RCT AV 774217-06-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

10/ 562,112

RGT D 7732-18-5 Water
CON cooled

PRO CZ 774217-43-5
NTE chemoselective

RX(97) RCT CZ 774217-43-5, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EL 774217-81-1

RX(134) RCT AU 88-74-4, EL 774217-81-1

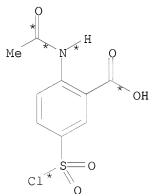
STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

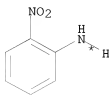
PRO FW 774218-15-4

RX(342) OF 372 COMPOSED OF RX(22), RX(60), RX(97), RX(134)

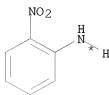
RX(342) A + 2 AU + DP ==> FW



A



AU

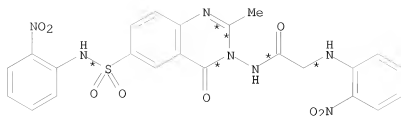


AU



DP

4
STEPS
→



FW
YIELD 65%

RX(22) RCT A 181478-44-4, AU 88-74-4

STAGE(1)
CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AV 774217-06-0

RX(60) RCT AV 774217-06-0

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO CZ 774217-43-5
NTE chemoselective

RX(97) RCT CZ 774217-43-5, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EL 774217-81-1

RX(134) RCT AU 88-74-4, EL 774217-81-1

STAGE(1)

10/ 562,112

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

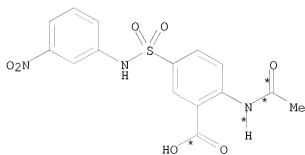
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO FW 774218-15-4

RX(343) OF 372 COMPOSED OF RX(61), RX(98), RX(135)

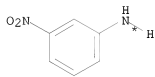
RX(343) AX + DP + AW ==> FX



AX

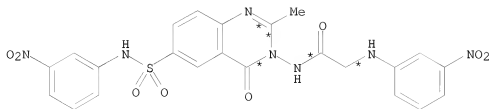


DP



AW

3
STEPS
→



FX
YIELD 63%

RX(61) RCT AX 774217-07-1

STAGE(1)

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RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DA 774217-44-6
NTE chemoselective

RX(98) RCT DA 774217-44-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EM 774217-82-2

RX(135) RCT AW 99-09-2, EM 774217-82-2

STAGE(1)

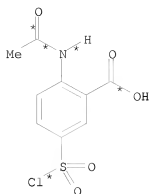
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

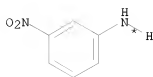
RGT D 7732-18-5 Water
CON cooled

PRO FX 774218-16-5

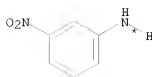
RX(344) OF 372 COMPOSED OF RX(23), RX(61), RX(98), RX(135)
RX(344) A + 2 AW + DP ==> FX



A



AW

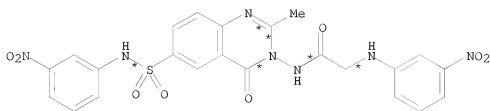


AW



DP

4
STEPS
→



FX

YIELD 63%

RX(23) RCT A 181478-44-4, AW 99-09-2

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO AX 774217-07-1

RX(61) RCT AX 774217-07-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
 SOL 67-56-1 MeOH
 CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO DA 774217-44-6
 NTE chemoselective

RX(98) RCT DA 774217-44-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO EM 774217-82-2

RX(135) RCT AW 99-09-2, EM 774217-82-2

STAGE(1)

RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

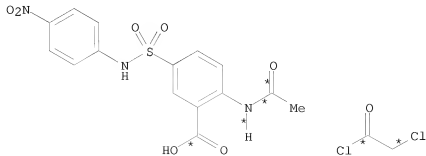
STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO FX 774218-16-5

RX(345) OF 372 COMPOSED OF RX(62), RX(99), RX(136)

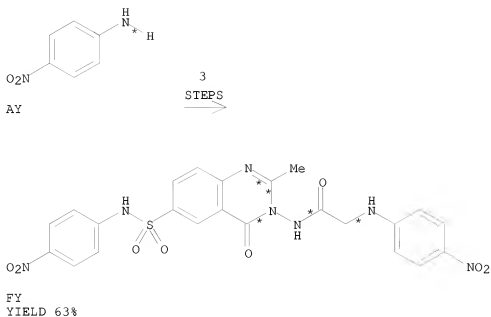
RX(345) AZ + DP + AY ==> FY



AZ

DP

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RX(62) RCT AZ 774217-08-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DB 774217-45-7
NTE chemoselective

RX(99) RCT DB 774217-45-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EN 774217-83-3

RX(136) RCT AY 100-01-6, EN 774217-83-3

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH

10/ 562,112

CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

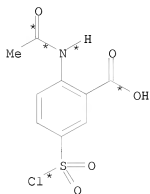
RGT D 7732-18-5 Water

CON cooled

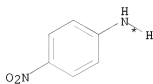
PRO FY 774218-17-6

RX(346) OF 372 COMPOSED OF RX(24), RX(62), RX(99), RX(136)

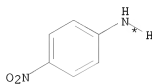
RX(346) A + 2 AY + DP ==> FY



A



AY

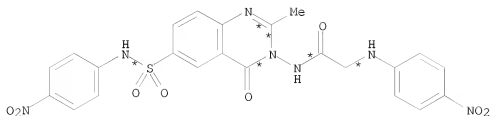


AY



DP

4
STEPS
→



FY

YIELD 63%

RX(24) RCT A 181478-44-4, AY 100-01-6

STAGE(1)

10/ 562,112

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO AZ 774217-08-2

RX(62) RCT AZ 774217-08-2

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DB 774217-45-7
NTE chemoselective

RX(99) RCT DB 774217-45-7, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EN 774217-83-3

RX(136) RCT AY 100-01-6, EN 774217-83-3

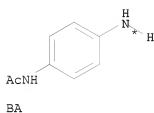
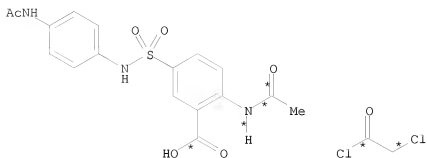
STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

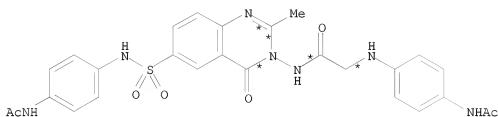
PRO FY 774218-17-6

RX(347) OF 372 COMPOSED OF RX(63), RX(100), RX(137)
RX(347) BB + DP + BA ==> FZ

10/ 562,112



3
STEPS
→



YIELD 53%

RX(63) RCT BB 774217-09-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DC 774217-46-8
NTE chemoselective

RX(100) RCT DC 774217-46-8, DP 79-04-9

STAGE(1)

10/ 562,112

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EO 774217-84-4

RX(137) RCT BA 122-80-5, EO 774217-84-4

STAGE(1)

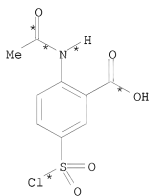
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

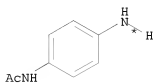
RGT D 7732-18-5 Water
CON cooled

PRO FZ 774218-18-7

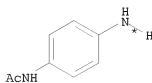
RX(348) OF 372 COMPOSED OF RX(25), RX(63), RX(100), RX(137)
RX(348) A + 2 BA + DP ==> FZ



A



BA

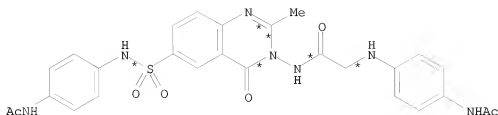


BA



DP

4
STEPS
➞



FZ
YIELD 53%

RX(25) RCT A 181478-44-4, BA 122-80-5

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BB 774217-09-3

RX(63) RCT BB 774217-09-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DC 774217-46-8
NTE chemoselective

RX(100) RCT DC 774217-46-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EO 774217-84-4

RX(137) RCT BA 122-80-5, EO 774217-84-4

STAGE(1)

10/ 562,112

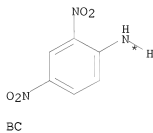
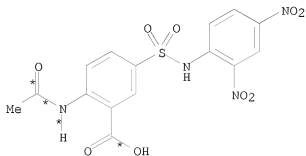
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

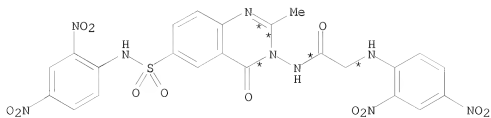
RGT D 7732-18-5 Water
CON cooled

PRO FZ 774218-18-7

RX(349) OF 372 COMPOSED OF RX(64), RX(101), RX(138)
RX(349) BD + DP + BC ==> GA



3
STEPS
=>



YIELD 61%

10/ 562,112

RX(64) RCT BD 774217-10-6

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DD 774217-47-9

NTE chemoselective

RX(101) RCT DD 774217-47-9, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EP 774217-85-5

RX(138) RCT BC 97-02-9, EP 774217-85-5

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

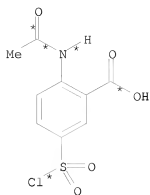
RGT D 7732-18-5 Water

CON cooled

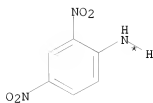
PRO GA 774218-19-8

RX(350) OF 372 COMPOSED OF RX(26), RX(64), RX(101), RX(138)

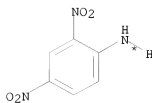
RX(350) A + 2 BC + DP ==> GA



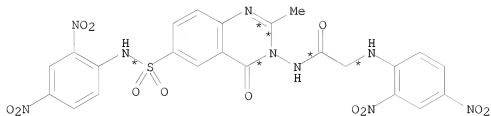
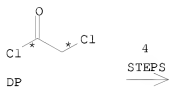
A



BC



BC



GA
YIELD 61%

RX(26) RCT A 181478-44-4, BC 97-02-9

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BD 774217-10-6

RX(64) RCT BD 774217-10-6

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DD 774217-47-9
NTE chemoselective

RX(101) RCT DD 774217-47-9, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EP 774217-85-5

RX(138) RCT BC 97-02-9, EP 774217-85-5

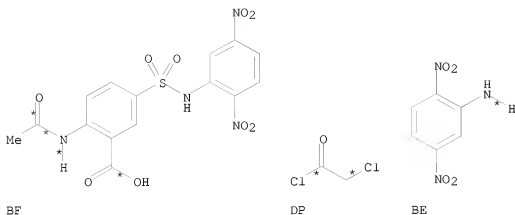
STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

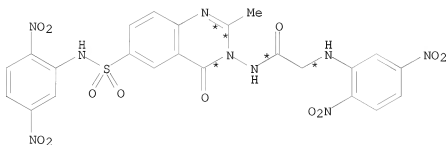
PRO GA 774218-19-8

RX(351) OF 372 COMPOSED OF RX(65), RX(102), RX(139)

RX(351) BF + DP + BE ==> GB



3
STEPS
→



GB
YIELD 63%

RX(65) RCT BF 774217-11-7

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DE 774217-48-0
NTE chemoselective

RX(102) RCT DE 774217-48-0, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EQ 774217-86-6

RX(139) RCT BE 619-18-1, EQ 774217-86-6

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

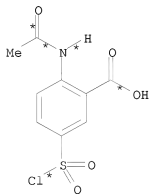
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

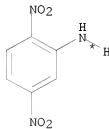
PRO GB 774218-20-1

RX(352) OF 372 COMPOSED OF RX(27), RX(65), RX(102), RX(139)

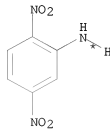
RX(352) A + 2 BE + DP ==> GB



A



BE

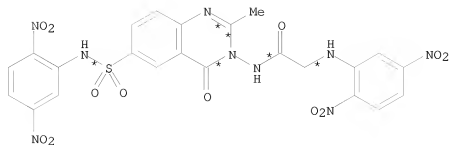


BE



DP

4
STEPS
→



GB
YIELD 63%

RX(27) RCT A 181478-44-4, BE 619-18-1

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BF 774217-11-7

RX(65) RCT BF 774217-11-7

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DE 774217-48-0

NTE chemoselective

RX(102) RCT DE 774217-48-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EQ 774217-86-6

RX(139) RCT BE 619-18-1, EQ 774217-86-6

STAGE(1)

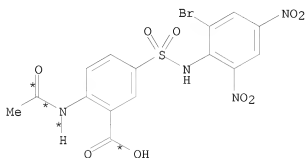
RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO GB 774218-20-1

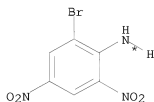
RX(353) OF 372 COMPOSED OF RX(66), RX(103), RX(140)
 RX(353) BH + DP + BG ==> GC



BH

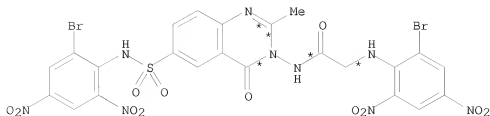


DP



BG

3
 STEPS
 →



GC
 YIELD 63%

RX(66) RCT BH 774217-12-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DF 774217-49-1
NTE chemoselective

RX(103) RCT DF 774217-49-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO ER 774217-87-7

RX(140) RCT BG 1817-73-8, ER 774217-87-7

STAGE(1)

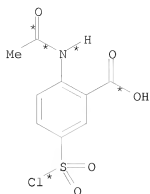
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

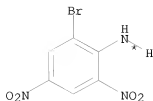
RGT D 7732-18-5 Water
CON cooled

PRO GC 774218-21-2

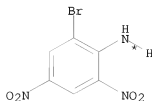
RX(354) OF 372 COMPOSED OF RX(28), RX(66), RX(103), RX(140)
RX(354) A + 2 BG + DP ==> GC



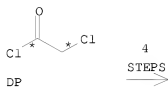
A



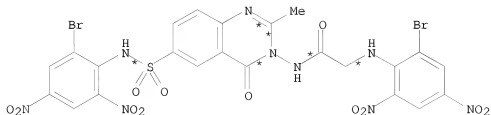
BG



BG



4
STEPS
→



GC
YIELD 63%

RX(28) RCT A 181478-44-4, BG 1817-73-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BH 774217-12-8

RX(66) RCT BH 774217-12-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
 SOL 67-56-1 MeOH
 CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO DF 774217-49-1
 NTE chemoselective

RX(103) RCT DF 774217-49-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO ER 774217-87-7

RX(140) RCT BG 1817-73-8, ER 774217-87-7

STAGE(1)

RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

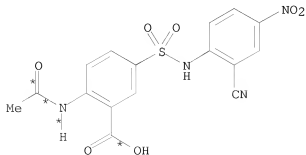
STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO GC 774218-21-2

RX(355) OF 372 COMPOSED OF RX(67), RX(104), RX(141)

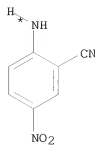
RX(355) BJ + DP + BI ==> GD



BJ



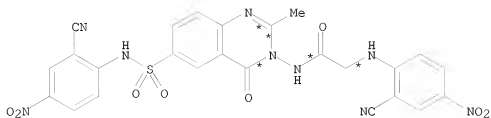
DP



BI

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3
STEPS
→



GD
YIELD 60%

RX(67) RCT BJ 774217-13-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DG 774217-50-4
NTE chemoselective

RX(104) RCT DG 774217-50-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO ES 774217-88-8

RX(141) RCT BI 17420-30-3, ES 774217-88-8

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

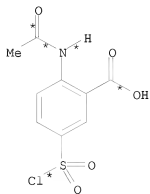
10/ 562,112

CON cooled

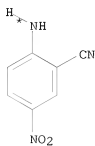
PRO GD 774218-22-3

RX(356) OF 372 COMPOSED OF RX(29), RX(67), RX(104), RX(141)

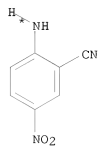
RX(356) A + 2 BI + DP ==> GD



A



BI

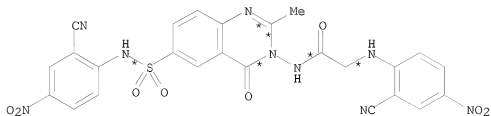


BI



DP

4
STEPS
=>



GD

YIELD 60%

RX(29) RCT A 181478-44-4, BI 17420-30-3

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BJ 774217-13-9

RX(67) RCT BJ 774217-13-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DG 774217-50-4

NTE chemoselective

RX(104) RCT DG 774217-50-4, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO ES 774217-88-8

RX(141) RCT BI 17420-30-3, ES 774217-88-8

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

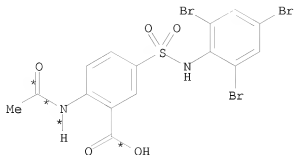
RGT D 7732-18-5 Water

CON cooled

PRO GD 774218-22-3

RX(357) OF 372 COMPOSED OF RX(68), RX(105), RX(142)

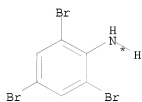
RX(357) BL + DP + BK ==> GE



BL

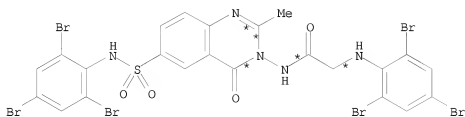


DP



BK

3
STEPS
→



GE

YIELD 65%

RX(68) RCT BL 774217-14-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DH 774217-51-5

NTE chemoselective

RX(105) RCT DH 774217-51-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO ET 774217-89-9

RX(142) RCT BK 147-82-0, ET 774217-89-9

STAGE(1)

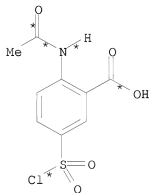
RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

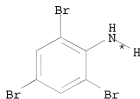
RGT D 7732-18-5 Water
 CON cooled

PRO GE 774218-23-4

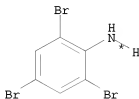
RX(358) OF 372 COMPOSED OF RX(30), RX(68), RX(105), RX(142)
 RX(358) A + 2 BK + DP ==> GE



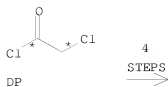
A



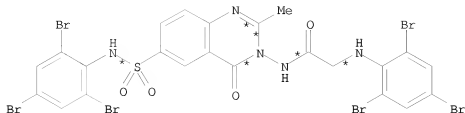
BK



BK



DP



GE
YIELD 65%

RX(30) RCT A 181478-44-4, BK 147-82-0

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BL 774217-14-0

RX(68) RCT BL 774217-14-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DH 774217-51-5
NTE chemoselective

RX(105) RCT DH 774217-51-5, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO ET 774217-89-9

RX(142) RCT BK 147-82-0, ET 774217-89-9

STAGE(1)

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RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

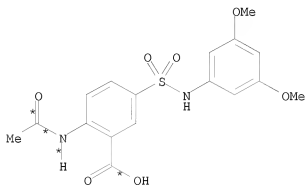
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO GE 774218-23-4

RX(359) OF 372 COMPOSED OF RX(69), RX(106), RX(143)

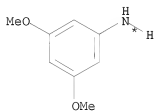
RX(359) BN + DP + BM ==> GF



BN

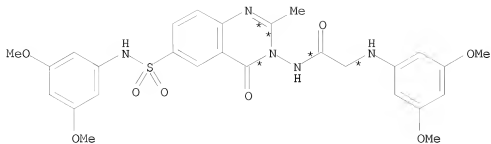


DP



BM

3
STEPS
➤



GF
YIELD 59%

RX(69) RCT BN 774217-15-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DI 774217-52-6
NTE chemoselective

RX(106) RCT DI 774217-52-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EU 774217-90-2

RX(143) RCT BM 10272-07-8, EU 774217-90-2

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

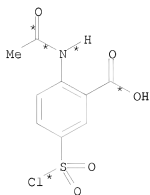
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

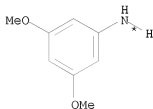
PRO GF 774218-24-5

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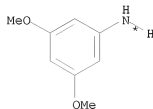
RX(360) OF 372 COMPOSED OF RX(31), RX(69), RX(106), RX(143)
 RX(360) A + 2 BM + DP ==> GF



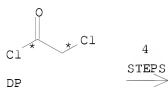
A



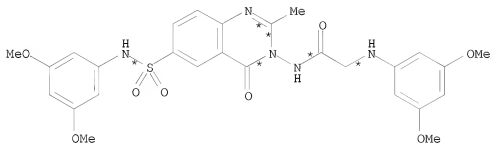
BM



BM



DP



GF
 YIELD 59%

RX(31) RCT A 181478-44-4, BM 10272-07-8

STAGE(1)

CAT 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO BN 774217-15-1

RX(69) RCT BN 774217-15-1

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DI 774217-52-6

NTE chemoselective

RX(106) RCT DI 774217-52-6, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EU 774217-90-2

RX(143) RCT BM 10272-07-8, EU 774217-90-2

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

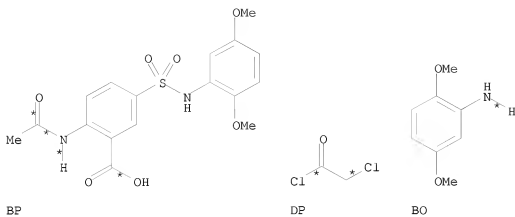
RGT D 7732-18-5 Water

CON cooled

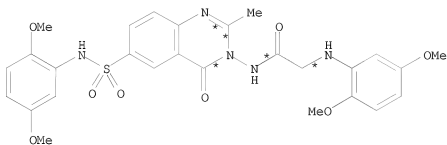
PRO GF 774218-24-5

RX(361) OF 372 COMPOSED OF RX(70), RX(107), RX(144)

RX(361) BP + DP + BO ==> GG



3
STEPS
→



GG
YIELD 60%

RX(70) RCT BP 774217-16-2

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DJ 774217-53-7
NTE chemoselective

RX(107) RCT DJ 774217-53-7, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH

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CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EV 774217-91-3

RX(144) RCT BO 102-56-7, EV 774217-91-3

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

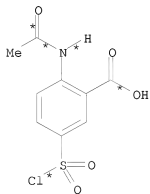
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

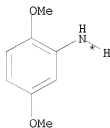
PRO GG 774218-25-6

RX(362) OF 372 COMPOSED OF RX(32), RX(70), RX(107), RX(144)

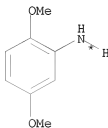
RX(362) A + 2 BO + DP ==> GG



A



BO

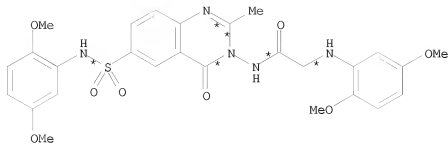


BO



DP

4
STEPS
→



GG
YIELD 60%

RX(32) RCT A 181478-44-4, BO 102-56-7

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BP 774217-16-2

RX(70) RCT BP 774217-16-2

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DJ 774217-53-7

NTE chemoselective

RX(107) RCT DJ 774217-53-7, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EV 774217-91-3

RX(144) RCT BO 102-56-7, EV 774217-91-3

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STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

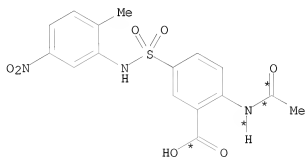
RGT D 7732-18-5 Water

CON cooled

PRO GG 774218-25-6

RX(363) OF 372 COMPOSED OF RX(71), RX(108), RX(145)

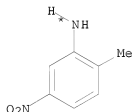
RX(363) BR + DP + BQ ==> GH



BR

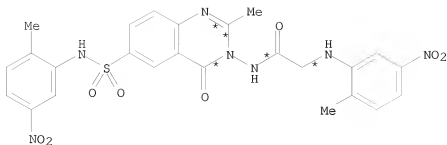


DP



BQ

3
STEPS
→



GH
YIELD 60%

RX(71) RCT BR 774217-17-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DK 774217-54-8
NTE chemoselective

RX(108) RCT DK 774217-54-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EW 774217-92-4

RX(145) RCT BQ 99-55-8, EW 774217-92-4

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

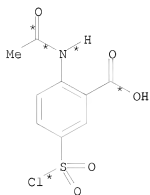
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

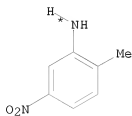
PRO GH 774218-26-7

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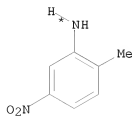
RX(364) OF 372 COMPOSED OF RX(33), RX(71), RX(108), RX(145)
 RX(364) A + 2 BQ + DP ==> GH



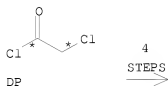
A



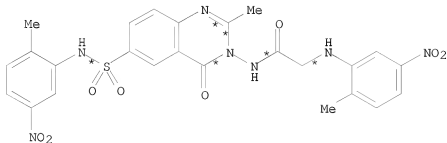
BQ



BQ



DP



GH

YIELD 60%

RX(33) RCT A 181478-44-4, BQ 99-55-8

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BR 774217-17-3

RX(71) RCT BR 774217-17-3

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DK 774217-54-8

NTE chemoselective

RX(108) RCT DK 774217-54-8, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EW 774217-92-4

RX(145) RCT BQ 99-55-8, EW 774217-92-4

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

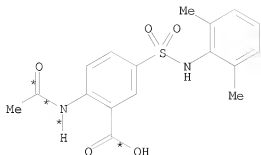
RGT D 7732-18-5 Water

CON cooled

PRO GH 774218-26-7

RX(365) OF 372 COMPOSED OF RX(72), RX(109), RX(147)

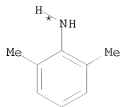
RX(365) BV + DP + BU ==> GK



BV

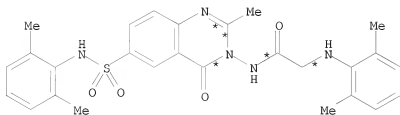


DP



BU

3
STEPS
→



GK
YIELD 57%

RX(72) RCT BV 774217-19-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DL 774217-56-0

NTE chemoselective

RX(109) RCT DL 774217-56-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

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RGT D 7732-18-5 Water
CON cooled

PRO EX 774217-94-6

RX(147) RCT BU 87-62-7, EX 774217-94-6

STAGE(1)

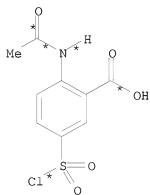
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

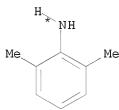
RGT D 7732-18-5 Water
CON cooled

PRO GK 774218-28-9

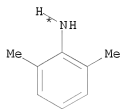
RX(366) OF 372 COMPOSED OF RX(35), RX(72), RX(109), RX(147)
RX(366) A + 2 BU + DP ==> GK



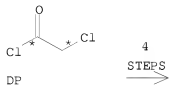
A



BU

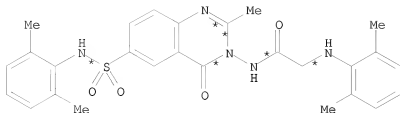


BU



DP

4
STEPS
→



GK

YIELD 57%

RX(35) RCT A 181478-44-4, BU 87-62-7

STAGE(1)

CAT 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO BV 774217-19-5

RX(72) RCT BV 774217-19-5

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DL 774217-56-0

NTE chemoselective

RX(109) RCT DL 774217-56-0, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO EX 774217-94-6

RX(147) RCT BU 87-62-7, EX 774217-94-6

STAGE(1)

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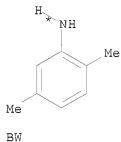
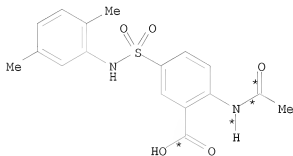
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

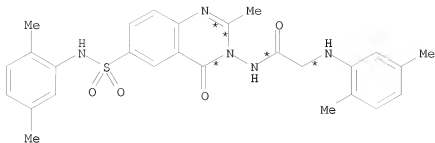
RGT D 7732-18-5 Water
CON cooled

PRO GK 774218-28-9

RX(367) OF 372 COMPOSED OF RX(73), RX(110), RX(148)
RX(367) BX + DP + BW ==> GL



3
STEPS
→



GL
YIELD 53%

RX(73) RCT BX 774217-20-8

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DM 774217-57-1
NTE chemoselective

RX(110) RCT DM 774217-57-1, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EY 774217-95-7

RX(148) RCT BW 95-78-3, EY 774217-95-7

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

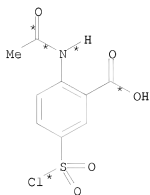
STAGE(2)

RGT D 7732-18-5 Water
CON cooled

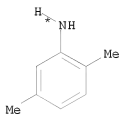
PRO GL 774218-29-0

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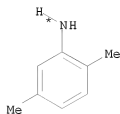
RX(368) OF 372 COMPOSED OF RX(36), RX(73), RX(110), RX(148)
 RX(368) A + 2 BW + DP ==> GL



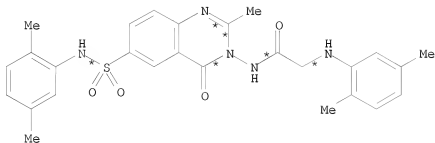
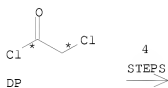
A



BW



BW



GL
 YIELD 53%

RX(36) RCT A 181478-44-4, BW 95-78-3

STAGE(1)

CAT 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO BX 774217-20-8

RX(73) RCT BX 774217-20-8

STAGE(1)
RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO DM 774217-57-1
NTE chemoselective

RX(110) RCT DM 774217-57-1, DP 79-04-9

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EY 774217-95-7

RX(148) RCT BW 95-78-3, EY 774217-95-7

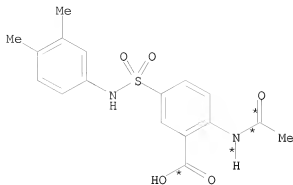
STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO GL 774218-29-0

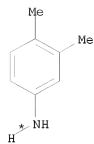
RX(369) OF 372 COMPOSED OF RX(74), RX(111), RX(149)
RX(369) BZ + DP + BY ==> GM

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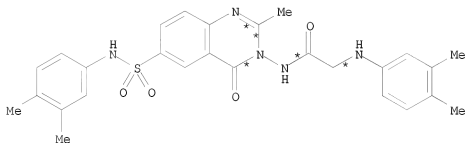
BZ

DP



BY

3
STEPS
→



GM
YIELD 53%

RX(74) RCT BZ 774217-21-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O

SOL 67-56-1 MeOH

CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DN 774217-58-2

NTE chemoselective

RX(111) RCT DN 774217-58-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

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SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO EZ 774217-96-8

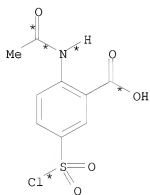
RX(149) RCT BY 95-64-7, EZ 774217-96-8

STAGE(1)
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

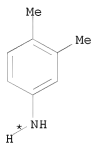
STAGE(2)
RGT D 7732-18-5 Water
CON cooled

PRO GM 774218-30-3

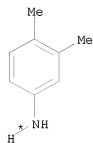
RX(370) OF 372 COMPOSED OF RX(37), RX(74), RX(111), RX(149)
RX(370) A + 2 BY + DP ==> GM



A



BY

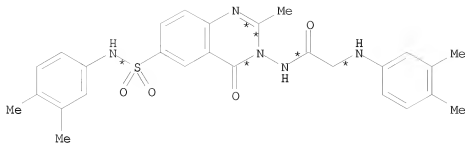


BY



DP

4
STEPS
→



GM
YIELD 53%

RX(37) RCT A 181478-44-4, BY 95-64-7

STAGE(1)

CAT 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO BZ 774217-21-9

RX(74) RCT BZ 774217-21-9

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH
CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO DN 774217-58-2

NTE chemoselective

RX(111) RCT DN 774217-58-2, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO EZ 774217-96-8

RX(149) RCT BY 95-64-7, EZ 774217-96-8

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STAGE(1)

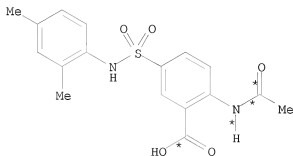
RGT E 110-86-1 Pyridine
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 4 hours, 120 deg C
SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
CON cooled

PRO GM 774218-30-3

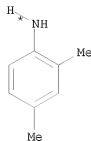
RX(371) OF 372 COMPOSED OF RX(75), RX(112), RX(150)
RX(371) CB + DP + CA ==> GN



CB

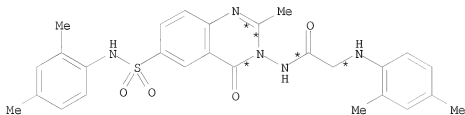


DP



CA

3
STEPS
→



GN
YIELD 65%

RX(75) RCT CB 774217-22-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
SOL 67-56-1 MeOH

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CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO DO 774217-59-3

NTE chemoselective

RX(112) RCT DO 774217-59-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO FA 774217-97-9

RX(150) RCT CA 95-68-1, FA 774217-97-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

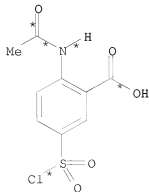
RGT D 7732-18-5 Water

CON cooled

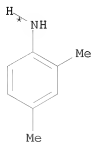
PRO GN 774218-31-4

RX(372) OF 372 COMPOSED OF RX(38), RX(75), RX(112), RX(150)

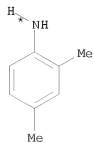
RX(372) A + 2 CA + DP ==> GN



A



CA

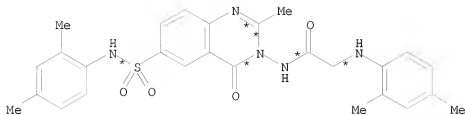


CA



DP

4
 STEPS
 →



GN
 YIELD 65%

RX(38) RCT A 181478-44-4, CA 95-68-1

STAGE(1)

CAT 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO CB 774217-22-0

RX(75) RCT CB 774217-22-0

STAGE(1)

RGT CD 7803-57-8 N2H4-H2O
 SOL 67-56-1 MeOH
 CON 3 hours, reflux

STAGE(2)

RGT D 7732-18-5 Water
 CON cooled

PRO DO 774217-59-3
 NTE chemoselective

RX(112) RCT DO 774217-59-3, DP 79-04-9

STAGE(1)

RGT E 110-86-1 Pyridine
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 120 deg C
 SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

10/ 562,112

CON cooled

PRO FA 774217-97-9

RX(150) RCT CA 95-68-1, FA 774217-97-9

STAGE(1)

RGT E 110-86-1 Pyridine

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 120 deg C

SUBSTAGE(2) cooled

STAGE(2)

RGT D 7732-18-5 Water

CON cooled

PRO GN 774218-31-4

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 67 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:325173 CASREACT

TITLE: Quinazolinone fungal efflux pump inhibitors. Part 2:

In vitro structure-activity relationships of
(N-methylpiperazinyl)-containing derivatives
AUTHOR(S): Watkins, William J.; Lemoine, Remy C.; Chong, Lee;
Cho, Aesop; Renau, Thomas E.; Kuo, Bonnie; Wong,
Vickie; Ludwikow, Maria; Garizi, Negar; Iqbal, Nadeem;
Barnard, John; Jankowska, Renata; Singh, Rajeshwar;
Madsen, Deidre; Lolans, Karen; Lomovskaya, Olga; Oza,
Uma; Dudley, Michael N.

CORPORATE SOURCE: Essential Therapeutics, Inc., Mountain View, CA,
94043, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004),
14(20), 5133-5137

CODEN: BMCLE8; ISSN: 0960-894X

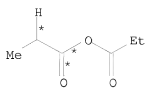
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

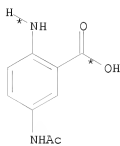
LANGUAGE: English

AB Structure-activity relationships of a novel series of fungal efflux pump
inhibitors with respect to potentiation of the activity of fluconazole
against strains of Candida albicans and Candida glabrata over-expressing
ABC-type efflux pumps are systematically explored.

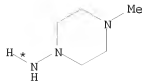
RX(45) OF 108 A + CR + C + F + X ==> CS



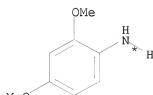
A



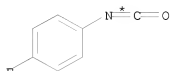
CR



C

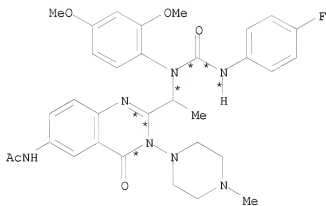


F



X

(45)



CS

RX (45) RCT A 123-62-6, CR 50670-83-2

STAGE (1)

CON 70 deg C

STAGE (2)

RCT C 6928-85-4

SOL 64-19-7 AcOH

CON 70 deg C

STAGE (3)

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RGT H 127-09-3 AcONa, I 7726-95-6 Br2
SOL 64-19-7 AcOH

STAGE(4)

RCT F 2735-04-8
SOL 872-50-4 NMEP
CON 80 deg C

STAGE(5)

RCT X 1195-45-5
SOL 107-06-2 ClCH2CH2Cl

PRO CS 770746-69-5

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 68 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:325172 CASREACT

TITLE: Quinazolinone-based fungal efflux pump inhibitors.
Part 1: Discovery of an
(N-methylpiperazine)-containing derivative with
activity in clinically relevant Candida spp.

AUTHOR(S): Lemoine, Remy C.; Glinka, Tomasz W.; Watkins, William
J.; Cho, Aesop; Yang, Jessie; Iqbal, Nadeem; Singh,
Rajeshwar; Madsen, Deidre; Lolans, Karen; Lomovskaya,
Olga; Oza, Uma; Dudley, Michael N.

CORPORATE SOURCE: Essential Therapeutics, Inc., Mountain View, CA,
94043, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004),
14(20), 5127-5131

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

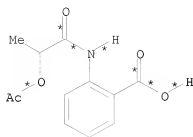
LANGUAGE: English

AB The discovery of a series of quinazolinone-based fungal efflux pump
inhibitors by high-throughput screening for potentiation of fluconazole in
C. albicans is described. Attempts to improve the aqueous solubility of
screening

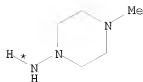
hits led to the discovery of an analog with greatly improved phys.
properties and activity against clin.-relevant Candida spp.

RX(17) OF 81 ...AJ + I ==> AM...

10/ 562,112

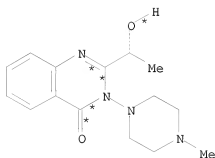


AJ



I

(17) \longrightarrow



AM

RX(17) RCT AJ 770743-64-1

STAGE(1)

RGT AA 108-24-7 Ac2O
CON 70 deg C

STAGE(2)

RCT I 6928-85-4
SOL 64-19-7 AcOH
CON 70 deg C

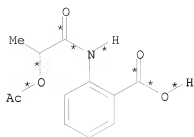
STAGE(3)

RGT AN 121-44-8 Et3N
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

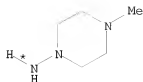
PRO AM 633305-72-3

RX(41) OF 81 COMPOSED OF RX(17), RX(18)

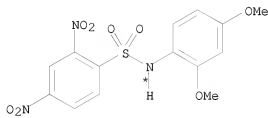
RX(41) AJ + I + AO ==> AP



AJ

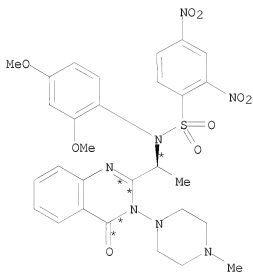


I



AO

2
STEPS
→



AP

RX(17) RCT AJ 770743-64-1

STAGE(1)

RGT AA 108-24-7 Ac2O

CON 70 deg C

STAGE(2)

RCT I 6928-85-4
SOL 64-19-7 AcOH
CON 70 deg C

STAGE(3)

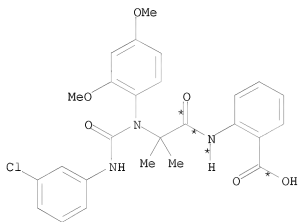
RGT AN 121-44-8 Et3N
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

PRO AM 633305-72-3

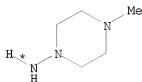
RX(18) RCT AM 633305-72-3, AO 633305-73-4
RGT AQ 603-35-0 PPh3, AR 2446-83-5 N2(CO2CHMe2)2
PRO AP 633305-74-5
SOL 109-99-9 THF
CON room temperature
NTE Mitsunobu reaction

RX(47) OF 81 COMPOSED OF RX(25), RX(26)

RX(47) BD + I ==> BF

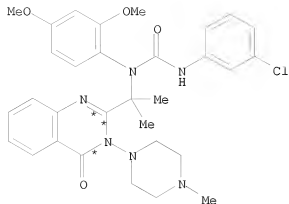


BD



I

2
STEPS
→

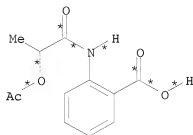


BF

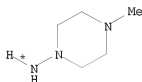
RX(25) RCT BD 770743-67-4
PRO BE 770743-68-5
SOL 108-24-7 Ac2O
CON 80 deg C

RX(26) RCT I 6928-85-4, BE 770743-68-5
PRO BF 770743-58-3
SOL 64-19-7 AcOH
CON 70 deg C

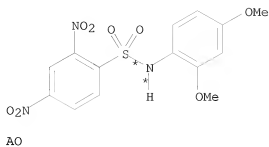
RX(66) OF 81 COMPOSED OF RX(17), RX(18), RX(19)
RX(66) AJ + I + AO ==> AT



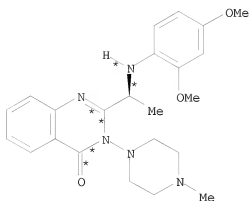
AJ



I



3
STEPS
→



RX(17) RCT AJ 770743-64-1

STAGE(1)

RGT AA 108-24-7 Ac2O
CON 70 deg C

STAGE(2)

RCT I 6928-85-4
SOL 64-19-7 AcOH
CON 70 deg C

STAGE(3)

RGT AN 121-44-8 Et3N
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

PRO AM 633305-72-3

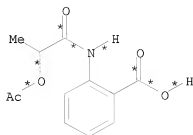
RX(18) RCT AM 633305-72-3, AO 633305-73-4
RGT AQ 603-35-0 PPh3, AR 2446-83-5 N2(CO2CHMe2)2
PRO AP 633305-74-5
SOL 109-99-9 THF
CON room temperature
NTE Mitsunobu reaction

RX(19) RCT AP 633305-74-5

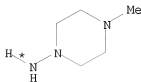
10/ 562,112

RGT AU 68-11-1 HSCH₂CO₂H, AN 121-44-8 Et₃N
PRO AT 633305-75-6
SOL 75-09-2 CH₂Cl₂
CON room temperature

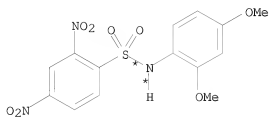
RX(69) OF 81 COMPOSED OF RX(17), RX(18), RX(19), RX(20)
RX(69) AJ + I + AO + V ==> AV



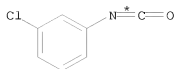
AJ



I

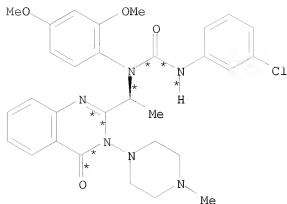


AO



V

4
STEPS
=>



AV

RX(17) RCT AJ 770743-64-1

STAGE(1)

RGT AA 108-24-7 Ac2O
CON 70 deg C

STAGE(2)

RCT I 6928-85-4
SOL 64-19-7 AcOH
CON 70 deg C

STAGE(3)

RGT AN 121-44-8 Et3N
SOL 7732-18-5 Water, 67-56-1 MeOH
CON room temperature

PRO AM 633305-72-3

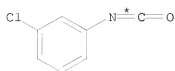
RX(18) RCT AM 633305-72-3, AO 633305-73-4
RGT AQ 603-35-0 PPh3, AR 2446-83-5 N2(CO2CHMe2)2
PRO AP 633305-74-5
SOL 109-99-9 THF
CON room temperature
NTE Mitsunobu reaction

RX(19) RCT AP 633305-74-5
RGT AU 68-11-1 HSCH2CO2H, AN 121-44-8 Et3N
PRO AT 633305-75-6
SOL 75-09-2 CH2Cl2
CON room temperature

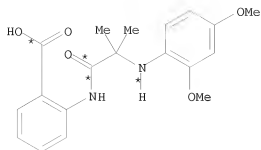
RX(20) RCT AT 633305-75-6, V 2909-38-8
PRO AV 770743-59-4
SOL 75-09-2 CH2Cl2
CON room temperature

RX(73) OF 81 COMPOSED OF RX(24), RX(25), RX(26)

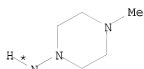
RX(73) V + BA + I ==> BF



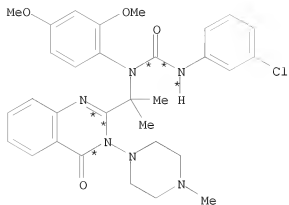
V



BA



I

3
STEPS

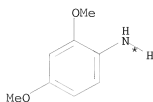
BF

RX(24) RCT V 2909-38-8, BA 770743-66-3
 PRO BD 770743-67-4
 SOL 75-09-2 CH2Cl2
 CON room temperature

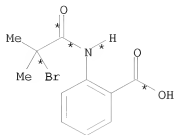
RX(25) RCT BD 770743-67-4
 PRO BE 770743-68-5
 SOL 108-24-7 Ac2O
 CON 80 deg C

RX(26) RCT I 6928-85-4, BE 770743-68-5
 PRO BF 770743-58-3
 SOL 64-19-7 AcOH
 CON 70 deg C

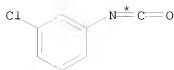
RX(74) OF 81 COMPOSED OF RX(23), RX(24), RX(25), RX(26)
 RX(74) P + AZ + V + I ==> BF



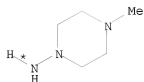
P



AZ

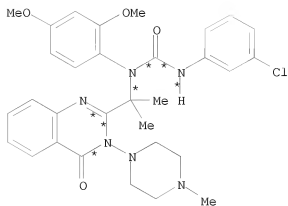


V



I

4
STEPS
→



BF

RX(23) RCT P 2735-04-8, AZ 770743-65-2
RGT BB 584-08-7 K2CO3
PRO BA 770743-66-3
SOL 64-17-5 EtOH
CON reflux

RX(24) RCT V 2909-38-8, BA 770743-66-3
PRO BD 770743-67-4
SOL 75-09-2 CH2Cl2
CON room temperature

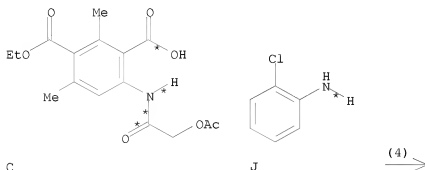
RX(25) RCT BD 770743-67-4
PRO BE 770743-68-5
SOL 108-24-7 Ac2O
CON 80 deg C

RX(26) RCT I 6928-85-4, BE 770743-68-5
PRO BF 770743-58-3
SOL 64-19-7 AcOH
CON 70 deg C

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 69 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 141:314290 CASREACT
 TITLE: A Facile Synthesis of
 C2,N3-Disubstituted-4-quinazolone
 AUTHOR(S): Xue, Song; McKenna, Joseph; Shieh, Wen-Chung; Repic,
 Oljan
 CORPORATE SOURCE: Chemical and Analytical Development, Novartis
 Institute for Biomedical Research, East Hanover, NJ,
 07936, USA
 SOURCE: Journal of Organic Chemistry (2004), 69(19), 6474-6477
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A simple and efficient methodol. for the synthesis of C2,N3-disubstituted
 4-quinazolones from anilines and N-acylanthranilic acids was developed.
 The new cyclization conditions are much milder than any other reported
 protocols and resulted in excellent yields (87-98%) without chromatog.

RX(4) OF 49 ...C + J ==> K...



K
 YIELD 95%

RX(4) RCT C 768368-41-8, J 95-51-2

STAGE(1)

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RGT L 7719-12-2 PC13
SOL 75-05-8 MeCN
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 50 deg C
SUBSTAGE(3) 2 hours, 50 deg C
SUBSTAGE(4) 50 deg C -> room temperature

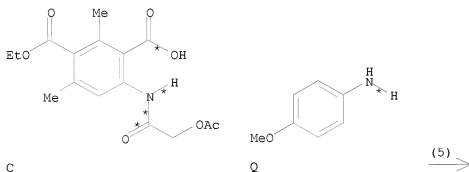
STAGE(2)

RGT M 7647-01-0 HCl
SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO K 768368-42-9

NTE optimization study, optimized on solvent

RX(5) OF 49 ...C + Q ==> R...



R
YIELD 94%

RX(5) RCT C 768368-41-8, Q 104-94-9

STAGE(1)

RGT L 7719-12-2 PC13
SOL 75-05-8 MeCN
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 50 deg C
SUBSTAGE(3) 2 hours, 50 deg C
SUBSTAGE(4) 50 deg C -> room temperature

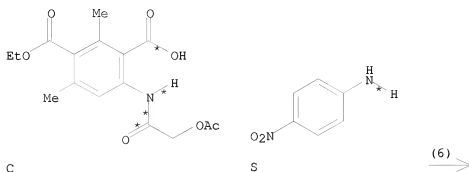
STAGE(2)

RGT M 7647-01-0 HCl
SOL 141-78-6 AcOEt, 7732-18-5 Water

10/ 562,112

PRO R 768368-43-0

RX(6) OF 49 ...C + S ==> T...



T
YIELD 96%

RX(6) RCT C 768368-41-8, S 100-01-6

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

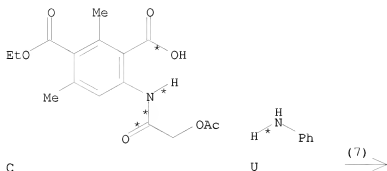
RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO T 768368-44-1

RX(7) OF 49 ...C + U ==> V...

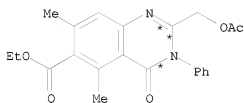
10/ 562,112



C

U

(7) →



V

YIELD 93%

RX(7) RCT C 768368-41-8, U 62-53-3

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

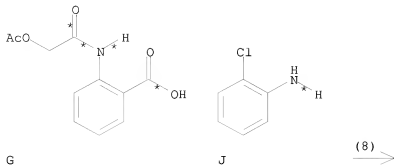
RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO V 77307-63-2

RX(8) OF 49 ...G + J ==> W...

10/ 562,112



W
YIELD 96%

RX(8) RCT G 51815-70-4, J 95-51-2

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

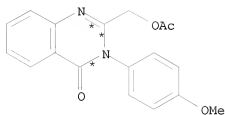
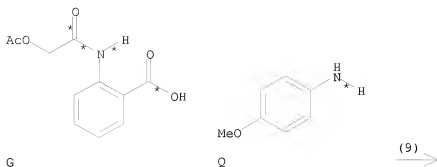
RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO W 54995-77-6

RX(9) OF 49 ...G + Q ==> X...

10/ 562,112



X
YIELD 97%

RX(9) RCT G 51815-70-4, Q 104-94-9

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

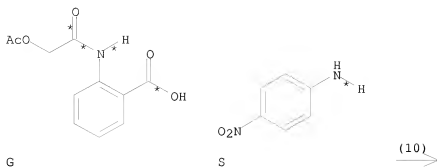
RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO X 768368-45-2

RX(10) OF 49 ...G + S ==> Y...

10/ 562,112



Y
YIELD 98%

RX(10) RCT G 51815-70-4, S 100-01-6

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

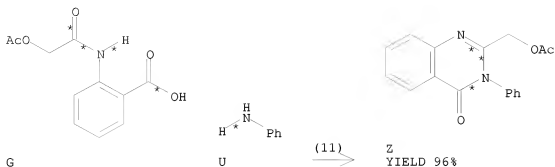
STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO Y 768368-46-3

RX(11) OF 49 ...G + U ==> Z...



RX(11) RCT G 51815-70-4, U 62-53-3

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

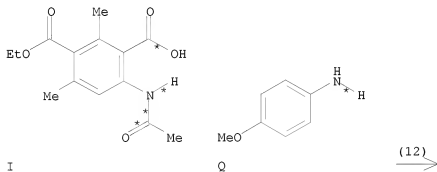
STAGE(2)

RGT M 7647-01-0 HCl

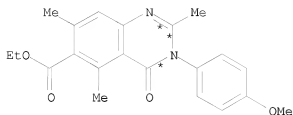
SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO Z 20873-19-2

RX(12) OF 49 ...I + Q ==> AA



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AA
YIELD 90%

RX(12) RCT I 75958-37-1, Q 104-94-9

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 20 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

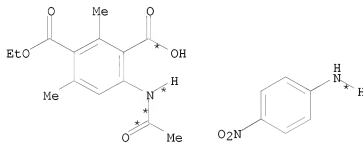
STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO AA 768368-47-4

RX(13) OF 49 ...I + S ==> AB

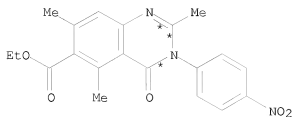


I

S

(13)
→

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AB
YIELD 96%

RX(13) RCT I 75958-37-1, S 100-01-6

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

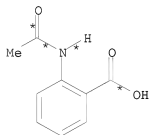
STAGE(2)

RGT M 7647-01-0 HCl

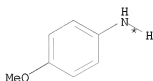
SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO AB 768368-48-5

RX(14) OF 49 AC + Q ==> AD



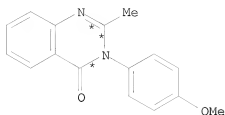
AC



Q

(14)
→

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AD
YIELD 87%

RX(14) RCT AC 89-52-1, Q 104-94-9

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 20 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

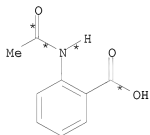
STAGE(2)

RGT M 7647-01-0 HCl

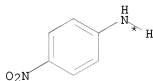
SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO AD 30507-16-5

RX(15) OF 49 AC + S ==> AE



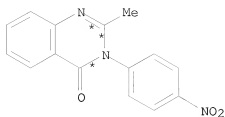
AC



S

(15)
→

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AE
YIELD 89%

RX(15) RCT AC 89-52-1, S 100-01-6

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 20 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

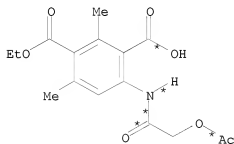
RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

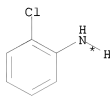
PRO AE 1788-96-1

RX(34) OF 49 COMPOSED OF RX(4), RX(16)

RX(34) C + J ==> AF



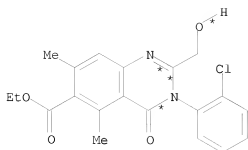
C



J

2
STEPS
→

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AF
YIELD 95%

RX(4) RCT C 768368-41-8, J 95-51-2

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO K 768368-42-9

NIE optimization study, optimized on solvent

RX(16) RCT K 768368-42-9

RGT AG 584-08-7 K2CO3

PRO AF 75913-83-6

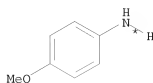
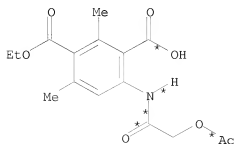
SOL 67-56-1 MeOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 20 minutes, room temperature

RX(35) OF 49 COMPOSED OF RX(5), RX(17)

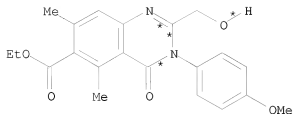
RX(35) C + Q ==> AI



C

Q

2
STEPS
→



● HCl

AI

YIELD 90%

RX(5) RCT C 768368-41-8, Q 104-94-9

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO R 768368-43-0

RX(17) RCT R 768368-43-0

STAGE(1)

RGT AG 584-08-7 K2CO3

SOL 67-56-1 MeOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 20 minutes, room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 7732-18-5 Water

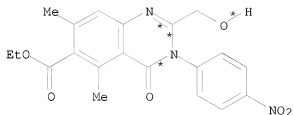
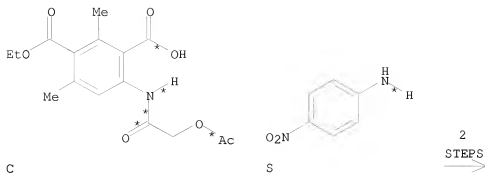
CON room temperature

PRO AI 768368-49-6

RX(36) OF 49 COMPOSED OF RX(6), RX(18)

RX(36) C + S ==> AJ

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AJ
YIELD 95%

RX(6) RCT C 768368-41-8, S 100-01-6

STAGE(1)

RGT L 7719-12-2 PC13
SOL 75-05-8 MeCN
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 50 deg C
SUBSTAGE(3) 2 hours, 50 deg C
SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl
SOL 141-78-6 AcOEt, 7732-18-5 Water

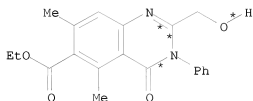
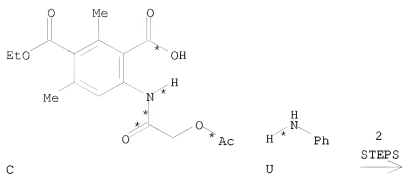
PRO T 768368-44-1

RX(18) RCT T 768368-44-1
RGT AG 584-08-7 K2CO3
PRO AJ 768368-50-9
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 20 minutes, room temperature

RX(37) OF 49 COMPOSED OF RX(7), RX(19)

RX(37) C + U ==> AK

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AK
YIELD 96%

RX(7) RCT C 768368-41-8, U 62-53-3

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO V 77307-63-2

RX(19)

RCT V 77307-63-2

RGT AG 584-08-7 K2CO3

PRO AK 77307-64-3

SOL 67-56-1 MeOH

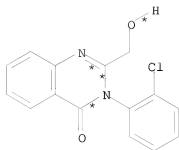
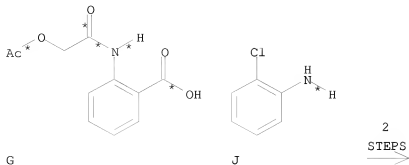
CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 20 minutes, room temperature

RX(38) OF 49 COMPOSED OF RX(8), RX(20)

RX(38) G + J ==> AL

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AL
YIELD 95%

RX(8) RCT G 51815-70-4, J 95-51-2

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO W 54995-77-6

RX(20)

RCT W 54995-77-6

RGT AG 584-08-7 K2CO3

PRO AL 29909-21-5

SOL 67-56-1 MeOH

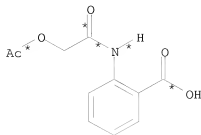
CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 20 minutes, room temperature

RX(39) OF 49 COMPOSED OF RX(9), RX(21)

RX(39) G + Q ==> AM

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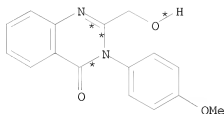


G



Q

2
STEPS
→



AM

YIELD 90%

RX(9) RCT G 51815-70-4, Q 104-94-9

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO X 768368-45-2

RX(21)

RCT X 768368-45-2

RGT AG 584-08-7 K2CO3

PRO AM 53615-54-6

SOL 67-56-1 MeOH

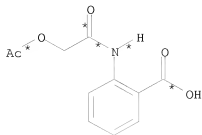
CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 20 minutes, room temperature

RX(40) OF 49 COMPOSED OF RX(10), RX(22)

RX(40) G + S ==> AN

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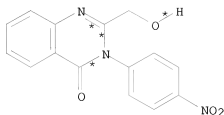


G



S

2
STEPS
→



AN

YIELD 91%

RX(10) RCT G 51815-70-4, S 100-01-6

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO Y 768368-46-3

RX(22) RCT Y 768368-46-3

RGT AG 584-08-7 K2CO3

PRO AN 768368-51-0

SOL 67-56-1 MeOH

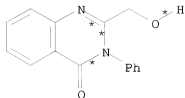
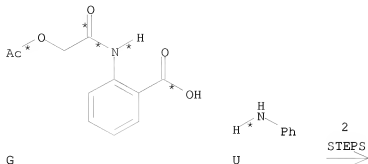
CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 20 minutes, room temperature

RX(41) OF 49 COMPOSED OF RX(11), RX(23)

RX(41) G + U ==> AO

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AO
YIELD 91%

RX(11) RCT G 51815-70-4, U 62-53-3

STAGE(1)

RGT L 7719-12-2 PC13

SOL 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

SUBSTAGE(3) 2 hours, 50 deg C

SUBSTAGE(4) 50 deg C -> room temperature

STAGE(2)

RGT M 7647-01-0 HCl

SOL 141-78-6 AcOEt, 7732-18-5 Water

PRO Z 20873-19-2

RX(23)

RCT Z 20873-19-2

RGT AG 584-08-7 K2CO3

PRO AO 20873-20-5

SOL 67-56-1 MeOH

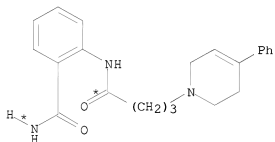
CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 20 minutes, room temperature

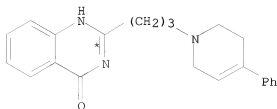
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 141:288542 CASREACT
 TITLE: Rational Approaches to Discovery of Orally Active and Brain-Penetrable Quinazolinone Inhibitors of Poly(ADP-ribose)polymerase
 AUTHOR(S): Hattori, Kouji; Kido, Yoshiyuki; Yamamoto, Hirofumi; Ishida, Junya; Kamijo, Kazunori; Murano, Kenji; Ohkubo, Mitsuru; Kinoshita, Takayoshi; Iwashita, Akinori; Mihara, Kayoko; Yamazaki, Syunji; Matsuoka, Nobuya; Teramura, Yoshinori; Miyake, Hiroshi
 CORPORATE SOURCE: Medicinal Chemistry Research Laboratories, Exploratory Research Laboratories, Medicinal Biology Research Laboratories, and Biopharmaceutical and Pharmacokinetic Research Laboratories, Fujisawa Pharmaceutical Co., Ltd., Osaka, 532-8514, Japan
 SOURCE: Journal of Medicinal Chemistry (2004), 47(17), 4151-4154
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A novel class of quinazolinone derivs. as potent poly(ADP-ribose)polymerase-1 (PARP-1) inhibitors has been discovered. Key to success was application of a rational discovery strategy involving structure-based design, combinatorial chemical, and classical SAR for improvement of potency and bioavailability. The new inhibitors were shown to bind to the nicotinamide-ribose binding site (NI site) and the adenosine-ribose binding site (AD site) of NAD+.

RX(32) OF 35 ...BR ==> D



BR

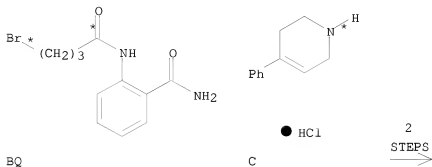


D
 YIELD 73%

RX(32) RCT BR 437998-41-9
 RGT J 1310-73-2 NaOH
 PRO D 437995-37-4
 SOL 7732-18-5 Water, 123-91-1 Dioxane
 CON 15 hours, room temperature
 NTE alternate solid-supported preparation also described, other
 analogs similarly prepared

RX(34) OF 35 COMPOSED OF RX(31), RX(32)

RX(34) BQ + C ==> D



D
 YIELD 73%

RX(31) RCT BQ 437998-35-1, C 43064-12-6

STAGE(1)

RGT BS 121-44-8 Et3N
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 0 deg C -> room temperature
 SUBSTAGE(2) 24 hours, room temperature

STAGE(2)

RGT N 7732-18-5 Water
 CON room temperature

PRO BR 437998-41-9

RX(32) RCT BR 437998-41-9
 RGT J 1310-73-2 NaOH

PRO D 437995-37-4
 SOL 7732-18-5 Water, 123-91-1 Dioxane
 CON 15 hours, room temperature
 NTE alternate solid-supported preparation also described, other analogs similarly prepared

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 71 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:225440 CASREACT

TITLE: Synthesis of some quinazolinone derivatives as possible anticancer agents

AUTHOR(S): Murugan, V.; Padmavathy, N. P.; Ramasarma, G. V. S.; Sharma, Sunil V.; Suresh, B.

CORPORATE SOURCE: Department of Pharmaceutical Chemistry, JSS College of Pharmacy, Ooty, 643 001, India

SOURCE: Indian Journal of Heterocyclic Chemistry (2003), 13(2), 143-146

CODEN: IJCHEI; ISSN: 0971-1627

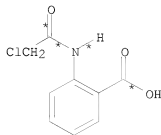
PUBLISHER: Prof. R. S. Varma

DOCUMENT TYPE: Journal

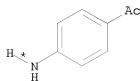
LANGUAGE: English

AB The title compds. 4-Chloro-1-[4-(6,8-disubstituted-2-chloromethyl-quinazolin-4-one-3-yl)-phenyl]butane-1,3-dione derivs. were synthesized by the reaction of corresponding 2-chloromethyl-3-(acetophenon-4-yl)-4-(3H)quinazolinone with Et chloroacetate in diisopropylether and NaOMe in dry methanol. Compound 2-(N-morpholinomethyl)-3-(acetophenon-4-yl)-4-(3H)quinazolinone was prepared by the reaction of 2-chloromethyl-3-(acetophenon-4-yl)-4-(3H)quinazolinone and morpholine in the presence of potassium carbonate in dry methanol. The intermediates N-chloroacetyl anthranilic acid derivs. and 2-chloromethyl-3-(acetophenon-4-yl)-4-(3H)quinazolinones were prepared by standard procedures. All the intermediates and title compds. were characterized by phys., chemical, anal. and spectral data. The biol. evaluation of the compds. was carried out by various methods such as short term study for in-vitro antitumor activity, cytostatic activity and antioxidant activity. Compds. 4-Chloro-1-[4-(6,8-dibromo-, 6,8-dichloro-, and 6-iodo-substituted-2-chloromethyl-quinazolin-4-one-3-yl)-phenyl]butane-1,3-diones showed significant anticancer activity.

RX(1) OF 17 A + B ==> C...



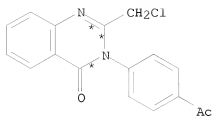
A



B



(1) →



C
YIELD 52%

RX(1) RCT A 14422-49-2, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

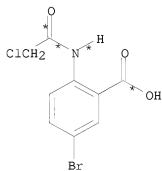
RGT E 144-55-8 NaHCO3

SOL 7732-18-5 Water

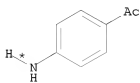
CON neutralized

PRO C 748165-98-2

RX(2) OF 17 H + B ==> I...



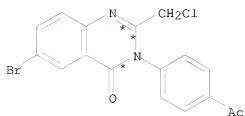
H



B

(2) >

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I
YIELD 69%

RX(2) RCT H 155104-20-4, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

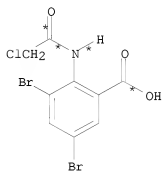
RGT E 144-55-8 NaHCO3

SOL 7732-18-5 Water

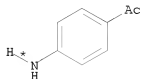
CON neutralized

PRO I 748165-99-3

RX(3) OF 17 J + B ==> K...



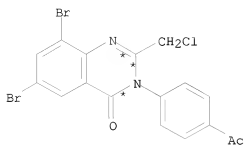
J



B

(3) >

10/ 562,112



K
YIELD 51%

RX(3) RCT J 103952-88-1, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PCl_3

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

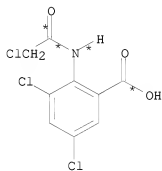
RGT E 144-55-8 NaHCO_3

SOL 7732-18-5 Water

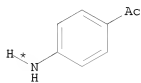
CON neutralized

PRO K 748166-00-9

RX(4) OF 17 L + B ==> M...



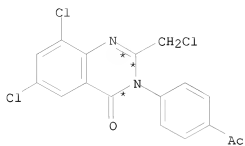
L



B

(4) >

10/ 562,112



M
YIELD 66%

RX(4) RCT L 39263-98-4, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

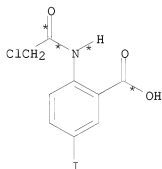
RGT E 144-55-8 NaHCO3

SOL 7732-18-5 Water

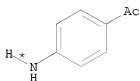
CON neutralized

PRO M 748166-01-0

RX(5) OF 17 N + B ==> O...



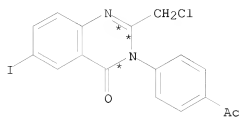
N



B

(5) >

10/ 562,112



O
YIELD 71%

RX(5) RCT N 175850-45-0, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT E 144-55-8 NaHCO3

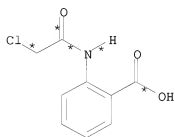
SOL 7732-18-5 Water

CON neutralized

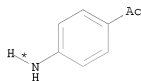
PRO O 748166-02-1

RX(12) OF 17 COMPOSED OF RX(1), RX(6)

RX(12) A + B + P ==> Q



A

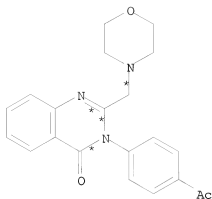


B



P

2
STEPS
→



Q
YIELD 70%

RX(1) RCT A 14422-49-2, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT E 144-55-8 NaHCO3

SOL 7732-18-5 Water

CON neutralized

PRO C 748165-98-2

RX(6) RCT C 748165-98-2, P 110-91-8

RGT R 584-08-7 K2CO3

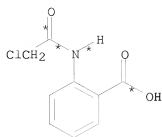
PRO Q 748166-08-7

SOL 67-56-1 MeOH

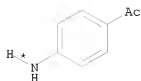
CON 4 hours, reflux

RX(13) OF 17 COMPOSED OF RX(1), RX(11)

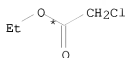
RX(13) A + B + T ==> AC



A

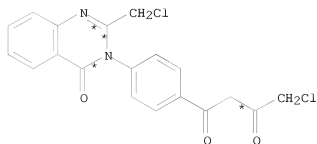


B



T

2
STEPS
→



AC
YIELD 58%

RX(1) RCT A 14422-49-2, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT E 144-55-8 NaHCO3

SOL 7732-18-5 Water

CON neutralized

PRO C 748165-98-2

RX(11) RCT T 105-39-5

STAGE(1)

RGT V 124-41-4 NaOMe

SOL 67-56-1 MeOH, 108-20-3 Isopropyl ether

CON 5 minutes, room temperature

STAGE(2)

RCT C 748165-98-2

SOL 108-20-3 Isopropyl ether

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CON SUBSTAGE(1) 5 minutes, room temperature
SUBSTAGE(2) 24 hours, reflux

STAGE(3)

RGT W 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(4)

RGT X 497-19-8 Na2CO3

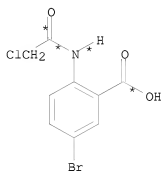
SOL 7732-18-5 Water

CON neutralized

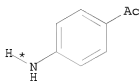
PRO AC 748166-03-2

RX(14) OF 17 COMPOSED OF RX(2), RX(7)

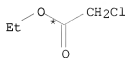
RX(14) H + B + T ==> U



H

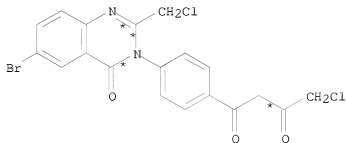


B



T

2
STEPS
→



U
YIELD 67%

RX(2) RCT H 155104-20-4, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13
SOL 108-88-3 PhMe
CON 3 hours, reflux

STAGE(2)
SOL 7732-18-5 Water

STAGE(3)
RGT E 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON neutralized

PRO I 748165-99-3

RX(7) RCT T 105-39-5

STAGE(1)
RGT V 124-41-4 NaOMe
SOL 67-56-1 MeOH, 108-20-3 Isopropyl ether
CON 5 minutes, room temperature

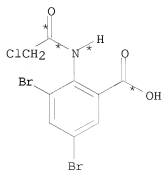
STAGE(2)
RCT I 748165-99-3
SOL 108-20-3 Isopropyl ether
CON SUBSTAGE(1) 5 minutes, room temperature
SUBSTAGE(2) 24 hours, reflux

STAGE(3)
RGT W 7647-01-0 HCl
SOL 7732-18-5 Water

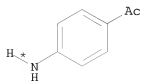
STAGE(4)
RGT X 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON neutralized

PRO U 748166-04-3

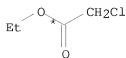
RX(15) OF 17 COMPOSED OF RX(3), RX(8)
RX(15) J + B + T ==> Z



J



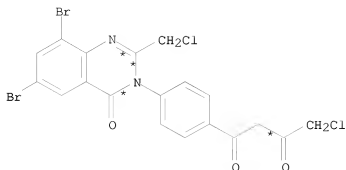
B



T

10/ 562,112

2
STEPS
→



Z
YIELD 52%

RX(3) RCT J 103952-88-1, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13

SOL 108-88-3 PhMe

CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT E 144-55-8 NaHCO₃

SOL 7732-18-5 Water

CON neutralized

PRO K 748166-00-9

RX(8) RCT T 105-39-5

STAGE(1)

RGT V 124-41-4 NaOMe

SOL 67-56-1 MeOH, 108-20-3 Isopropyl ether

CON 5 minutes, room temperature

STAGE(2)

RCT K 748166-00-9

SOL 108-20-3 Isopropyl ether

CON SUBSTAGE(1) 5 minutes, room temperature

SUBSTAGE(2) 24 hours, reflux

STAGE(3)

RGT W 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(4)

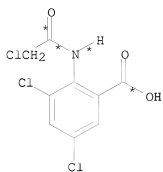
RGT X 497-19-8 Na₂CO₃

10/ 562,112

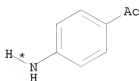
SOL 7732-18-5 Water
CON neutralized

PRO Z 748166-05-4

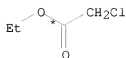
RX(16) OF 17 COMPOSED OF RX(4), RX(9)
RX(16) L + B + T ==> AA



L

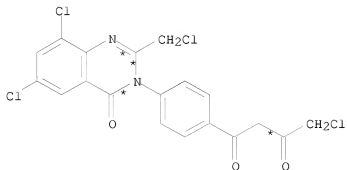


B



T

2
STEPS
→



AA
YIELD 49%

RX(4) RCT L 39263-98-4, B 99-92-3

STAGE(1)
RGT D 7719-12-2 PC13
SOL 108-88-3 PhMe
CON 3 hours, reflux

STAGE(2)
SOL 7732-18-5 Water

10/ 562,112

STAGE(3)

RGT E 144-55-8 NaHCO3

SOL 7732-18-5 Water

CON neutralized

PRO M 748166-01-0

RX(9) RCT T 105-39-5

STAGE(1)

RGT V 124-41-4 NaOMe

SOL 67-56-1 MeOH, 108-20-3 Isopropyl ether

CON 5 minutes, room temperature

STAGE(2)

RCT M 748166-01-0

SOL 108-20-3 Isopropyl ether

CON SUBSTAGE(1) 5 minutes, room temperature

SUBSTAGE(2) 24 hours, reflux

STAGE(3)

RGT W 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(4)

RGT X 497-19-8 Na2CO3

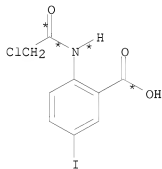
SOL 7732-18-5 Water

CON neutralized

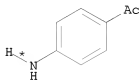
PRO AA 748166-06-5

RX(17) OF 17 COMPOSED OF RX(5), RX(10)

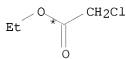
RX(17) N + B + T ==> AB



N

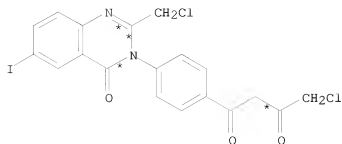


B



T

2
STEPS
→



AB
YIELD 63%

RX(5) RCT N 175850-45-0, B 99-92-3

STAGE(1)

RGT D 7719-12-2 PC13
SOL 108-88-3 PhMe
CON 3 hours, reflux

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT E 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON neutralized

PRO O 748166-02-1

RX(10) RCT T 105-39-5

STAGE(1)

RGT V 124-41-4 NaOMe
SOL 67-56-1 MeOH, 108-20-3 Isopropyl ether
CON 5 minutes, room temperature

STAGE(2)

RCT O 748166-02-1
SOL 108-20-3 Isopropyl ether
CON SUBSTAGE(1) 5 minutes, room temperature
SUBSTAGE(2) 24 hours, reflux

STAGE(3)

RGT W 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(4)

RGT X 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON neutralized

PRO AB 748166-07-6

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 72 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 141:225304 CASREACT
 TITLE: Preparation of cyclohexyl-substituted lactams as cytokine receptor modulating agents
 INVENTOR(S): Cherney, Robert J.; Carter, Percy; Duncia, John V.; Gardner, Daniel S.; Santella, Joseph B.
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
 SOURCE: PCT Int. Appl., 385 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

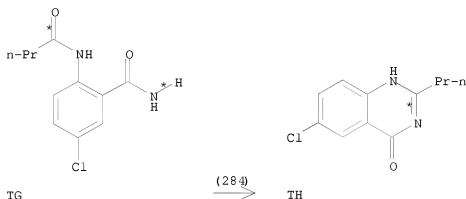
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
WO 2004071460	A2	20040826	WO 2004-US4418	20040211
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20040186140	A1	20040923	US 2004-776828	20040211
US 7183270	B2	20070227		
EP 1606255	A2	20051221	EP 2004-710294	20040211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 20070032541	A1	20070208	US 2006-545584	20061010
US 7338947	B2	20080304		
US 20080114052	A1	20080515	US 2008-18266	20080123
PRIORITY APPLN. INFO.:			US 2003-446850P	20030212
			US 2004-776828	20040211
			WO 2004-US4418	20040211
			US 2006-545584	20061010
OTHER SOURCE(S):		MARPAT 141:225304		
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Cyclohexyl-substituted lactams I [A = (un)substituted saturated or partially saturated cycloalkyl or heterocycloalkyl group with 3-8 atoms; E = S(:O)pCHR₃, CHR₃NR₃, C(:O)NR₃, N(R₃)C(:O)NR₃, SO₂N(R₃), N(R₃)SO₂N(R₃); G = (CHR₁₀)_n; J = CH₂CH₂, CH:CH un(substituted) with (R₁₃)_s; R₁, R₂ = (un)substituted aryl or heteroaryl ring; R₃ = H, alkyl; R₁₀ = H, (un)substituted alkyl (two R₁₀ groups may together comprise a carbonyl group); R₁₁, R₁₂ (independently) = H, (un)substituted alkyl, aralkyl, heteroaralkyl, s-hydroxyalkyl, s-mercaptoalkyl, s-alkoxyalkyl, etc.; R₁₃ = H, (un)substituted alkyl; X = O, S; Z = bond, (un)substituted aminocarbonyl, aminothiocarbonyl, aminocarbonylamino, aminothiocarbonylamino, aminosulfonyl, aminosulfonylamino, carbonylamino, oxycarbonylamino,

aminocarbonyloxy, alkenediyl, methylene, etc.; m = 0-1; n = 0-3; s = 0-1] such as II are prepared as modulators of cytokine activity for the treatment of diseases associated with cytokines and their receptors such as inflammation, osteo- and rheumatoid arthritis, autoimmune diseases, HIV infection, inflammatory bowel disease, asthma, multiple sclerosis, and atherosclerosis. E.g., 1,4-cyclohexanedione mono(ethylene ketal) is lithiated and acylated with Et cyanoformate, reductively aminated with (S)- α -methylbenzylamine, subjected to reduction with lithium aluminum hydride followed by hydrogenolysis with palladium hydroxide and protection with Cbz anhydride to yield nonracemic III. E.g., III undergoes substitution at the primary carbon with 4-bromophenyl disulfide and tributylphosphine followed by oxidation with mCPBA, Stille methylation of the p-bromophenyl moiety, hydrogenolysis of the Cbz protecting group, acylation with N-Cbz-L-methionine, and S-methylation and cyclization with Me iodide and cesium carbonate to yield IV. E.g., IV undergoes acid-catalyzed deketalization, titanium-mediated Meerwein-Pondorff-Verley reduction with isopropylamine (giving a mixture of both epimers at the amine center), N-methylation with formaldehyde and sodium triacetoxyborohydride, hydrogenolysis of the Cbz protecting group on the aminopyrrolidinone, and acylation with 3-trifluoromethylbenzoic acid and HATU to yield II. The compds. are modulators of chemokine receptor activity (no data). In addition, methods of halolactamization and dehalogenation and reagents appropriate for such transformations are claimed.

RX(284) OF 1483 ...TG ==> TH...



RX(284) RCT TG 746671-46-5

STAGE(1)

RGT BD 1310-73-2 NaOH
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 15 minutes, room temperature

STAGE(2)

RGT CL 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, pH 2

PRO TH 69729-73-3

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 73 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:106431 CASREACT

TITLE: Synthesis of 6-bromomethyl-3,4-dihydro-2-methyl-4-oxoquinazoline

AUTHOR(S): Cao, Sheng-li; Ma, Xue-qin

CORPORATE SOURCE: Department of Chemistry, Capital Normal University, Beijing, 100037, Peop. Rep. China

SOURCE: Huaxue Shiji (2004), 26(1), 27-28, 49

CODEN: HUSHDR; ISSN: 0258-3283

PUBLISHER: Huagongbu Huaxue Shiji Xinsizhan

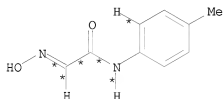
DOCUMENT TYPE: Journal

LANGUAGE: Chinese

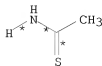
AB Cyclization of 4-MeC₆H₄NHCOCH:NOH with H₂SO₄ gave 5-methylisatin, oxidation of which with 30% H₂O₂ gave 2-amino-5-methylbenzoic acid. Then, heating 2-amino-5-methylbenzoic acid with thioacetamide yielded 3,4-dihydro-2,6-dimethyl-4-oxoquinazoline which was brominated with N-bromosuccinimide in the presence of benzoyl peroxide to give the title compound in 23.1% overall yield.

RX(8) OF 10 COMPOSED OF RX(1), RX(2), RX(3)

RX(8) A + I ==> J

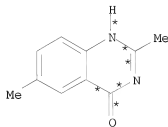


A



I

3
STEPS
➔



J

YIELD 73%

RX(1) RCT A 1132-40-7
RGT C 7664-93-9 H₂SO₄
PRO B 608-05-9

RX(2) RCT B 608-05-9

10/ 562,112

STAGE(1)

RGT E 7722-84-1 H2O2, F 1310-73-2 NaOH

SOL 7732-18-5 Water

CON 0.5 hours, 15 - 20 deg C

STAGE(2)

RGT G 7647-01-0 HCl

SOL 7732-18-5 Water

CON 0 deg C, pH 5 - 6

PRO D 2941-78-8

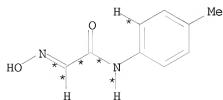
RX(3) RCT D 2941-78-8, I 62-55-5

PRO J 18731-19-6

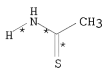
CON 2 hours, 135 - 150 deg C

RX(10) OF 10 COMPOSED OF RX(1), RX(2), RX(3), RX(4)

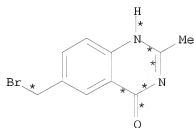
RX(10) A + I ==> K



A



I



K

YIELD 76%

RX(1) RCT A 1132-40-7

RGT C 7664-93-9 H2SO4

PRO B 608-05-9

RX(2) RCT B 608-05-9

STAGE(1)

RGT E 7722-84-1 H2O2, F 1310-73-2 NaOH

SOL 7732-18-5 Water

CON 0.5 hours, 15 - 20 deg C

STAGE(2)

RGT G 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON 0 deg C, pH 5 - 6

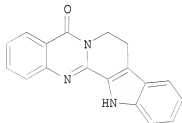
PRO D 2941-78-8

RX(3) RCT D 2941-78-8, I 62-55-5
 PRO J 18731-19-6
 CON 2 hours, 135 - 150 deg C

RX(4) RCT J 18731-19-6
 RGT L 128-08-5 Bromosuccinimide
 PRO K 112888-43-4
 CAT 94-36-0 Benzoyl peroxide
 SOL 67-66-3 CHCl3
 CON 3 hours, 60 - 62 deg C
 NTE photochem.

L3 ANSWER 74 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:23764 CASREACT
 TITLE: Facile zeolite induced Fischer-indole synthesis: a new approach to bioactive natural product rutaecarpine
 AUTHOR(S): Mhaske, Santosh B.; Argade, Narshinha P.
 CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National Chemical Laboratory, Pashan, Pune, 411 008, India
 SOURCE: Tetrahedron (2004), 60(15), 3417-3420
 CODEN: TETRAB; ISSN: 0040-4020
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

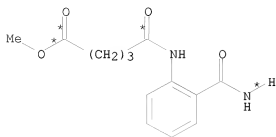


I

AB Starting from glutaric anhydride we have demonstrated an elegant six-step practical synthesis of bioactive natural product rutaecarpine (I) via o-amidoglutaranilic acid formation, esterification, chemoselective ester reduction, intramol. dehydrative cyclizations, hydrazone formation and zeolite induced Fischer-indole synthesis with 53% overall yield. The conditions employed in the present synthesis are mild, efficient and general.

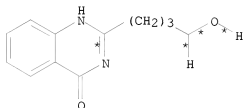
RX(3) OF 21 ...G ==> I...

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G

(3) \rightarrow



I

YIELD 86%

RX(3) RCT G 697236-30-9

STAGE(1)

RGT J 16940-66-2 NaBH4

SOL 109-99-9 THF

CON 3 hours, reflux

STAGE(2)

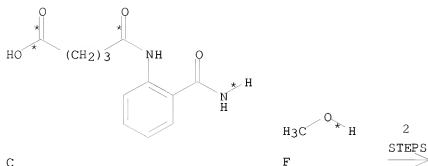
RGT K 7732-18-5 Water

CON room temperature

PRO I 60915-16-4

RX(8) OF 21 COMPOSED OF RX(2), RX(3)

RX(8) C + F ==> I



I
YIELD 86%

RX(2) RCT C 197236-49-0, F 67-56-1
PRO G 697236-30-9
CAT 7664-93-9 H2SO4
SOL 67-56-1 MeOH
CON 8 hours, room temperature

RX(3) RCT G 697236-30-9

STAGE(1)
RGT J 16940-66-2 NaBH4
SOL 109-99-9 THF
CON 3 hours, reflux

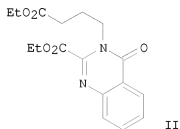
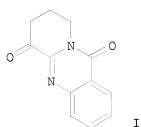
STAGE(2)
RGT K 7732-18-5 Water
CON room temperature

PRO I 60915-16-4

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

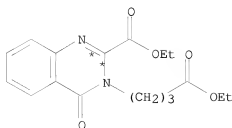
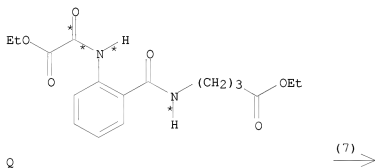
L3 ANSWER 75 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 141:7327 CASREACT
TITLE: A facile total synthesis of rutaecarpine
AUTHOR(S): Chavan, Subhash P.; Sivappa, R.
CORPORATE SOURCE: Division of Organic Chemistry: Technology, National

SOURCE: Chemical Laboratory, Pune, 411-008, India
 Tetrahedron Letters (2004), 45(5), 997-999
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The indoloquinazoline alkaloid rutaecarpine was synthesized efficiently by employing 9,10,11,12-tetrahydro-4H-pyrido[2,1-b]quinazoline-4,9-dione (I) as a key intermediate, which was prepared by adapting a Dieckmann condensation-decarboxylation sequence from quinazolinone diester II.

RX(7) OF 29 ...Q ==> H...

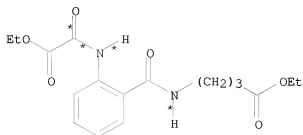


YIELD 80%

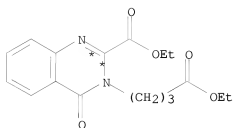
10/ 562,112

RX(7) RCT Q 693226-79-8
RGT T 7719-12-2 PC13
PRO H 107466-57-9
SOL 1330-20-7 Xylene
CON 2 hours, reflux

RX(8) OF 29 Q ==> H



Q



H
YIELD 70%

RX(8) RCT Q 693226-79-8

STAGE(1)

RGT V 603-35-0 PPh3, W 7553-56-2 I2, N 121-44-8 Et3N
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT X 110-89-4 Piperidine
SOL 75-05-8 MeCN
CON reflux

PRO H 107466-57-9

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 76 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 141:7091 CASREACT

TITLE: An interaction of 2-thiazoleacetonitriles with
N-(2-chloroacetyl)anthranilic acid esterAUTHOR(S): Resnyanska, Elizaveta V.; Tverdokhlebov, Anton V.;
Tolmachev, Andrey A.; Volovenko, Yulian M.; Shokol,
Tatyana V.

CORPORATE SOURCE: Enamine Ltd. Co., Kiev, 02042, Ukraine

SOURCE: Heterocycles (2004), 63(4), 797-807

CODEN: HTCYAM; ISSN: 0385-5414

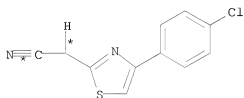
PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

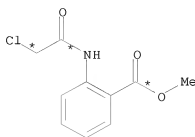
LANGUAGE: English

AB The title ester was found to react with 2-benzothiazoleacetonitrile yielding 3-(2-benzothiazolyl)-2,4-dihydropyrrolo[1,2-a]quinazoline-1,5-dione. At the same time 4-aryl-2-thiazoleacetonitriles gave 3,4-dihydro- β ,4-dioxo- α , δ -bis(4-aryl-2-thiazolyl)-2-quinazolinepentanenitriles potassium salts under identical conditions. These results were explained in terms of different solubility of the intermediate compds. Upon acidification the obtained salts were shown to undergo intramol. Thorpe addition leading to the 3-amino-2,4-bis(4-aryl-2-thiazolyl)-4-[4(3H)-oxo-2-quinazolinyl]-2-cyclopenten-1-ones. Above mentioned pyrrolo[1,2-a]quinazoline derivative was treated with benzylamines and active methylene nitriles to yield β -(2-benzothiazolyl)-N-arylmethyl-3,4-dihydro-4-oxo-2-quinazolinepropanamides and 2-substituted 3-amino-4-(2-benzothiazolyl)-4-[4(3H)-oxo-2-quinazolinyl]-2-cyclopenten-1-ones, resp.

RX(2) OF 15 2 F + B ==> G...



2 F



B



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(2) RCT F 17969-48-1, B 58915-18-7

RGT D 584-08-7 K2CO3

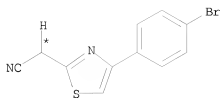
PRO G 694495-39-1

SOL 64-17-5 EtOH

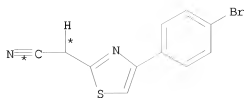
CON 1.5 hours, reflux

NTE Claisen type acylation

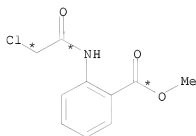
RX(3) OF 15 2 H + B ==> I...



H



H



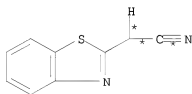
B



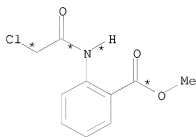
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(3) RCT H 94833-31-5, B 58915-18-7
 RGT D 584-08-7 K2CO3
 PRO I 694495-40-4
 SOL 64-17-5 EtOH
 CON 1.5 hours, reflux
 NTE Claisen type acylation

RX(12) OF 15 COMPOSED OF RX(1), RX(8)
 RX(12) A + B + S ==> T



A



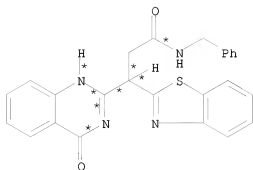
B



S

10/ 562,112

2
STEPS
→

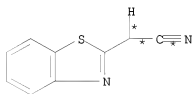


T
YIELD 54%

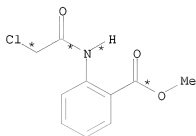
RX(1) RCT A 56278-50-3, B 58915-18-7
RGT D 584-08-7 K2CO3
PRO C 519048-05-6
SOL 64-17-5 EtOH
CON 1.5 hours, reflux

RX(8) RCT S 100-46-9, C 519048-05-6
PRO T 565179-87-5
SOL 68-12-2 DMF
CON 3 hours, 100 deg C

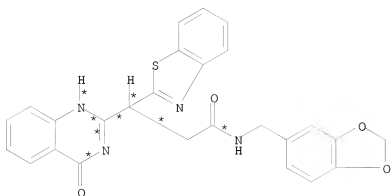
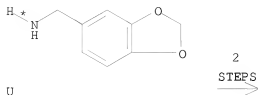
RX(13) OF 15 COMPOSED OF RX(1), RX(9)
RX(13) A + B + U ==> V



A



B



V
YIELD 56%

RX(1) RCT A 56278-50-3, B 58915-18-7
RGT D 584-08-7 K₂CO₃
PRO C 519048-05-6
SOL 64-17-5 EtOH
CON 1.5 hours, reflux

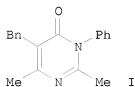
RX(9) RCT U 2620-50-0, C 519048-05-6
PRO V 568577-53-7
SOL 68-12-2 DMF
CON 3 hours, 100 deg C

REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 77 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 140:339284 CASREACT
TITLE: An efficient synthesis of 3-substituted
3H-pyrimidin-4-ones
AUTHOR(S): Jeong, Jae Uk; Chen, Xiaohong; Rahman, Attiq;
Yamashita, Dennis S.; Luengo, Juan I.
CORPORATE SOURCE: Department of Medicinal Chemistry, MMPD CEDD,
GlaxoSmithKline, Collegeville, PA, 19426, USA
SOURCE: Organic Letters (2004), 6(6), 1013-1016
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society

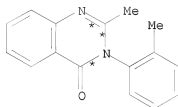
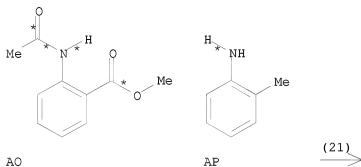
DOCUMENT TYPE:
LANGUAGE:
GI

Journal
English



AB A practical synthesis of 3-substituted 3H-pyrimidin-4-ones, e.g., I, is described. The key step involved the cyclization of enamide esters, derived from readily available β -keto esters, with various primary amines.

RX(21) OF 42 AO + AP ==> AQ



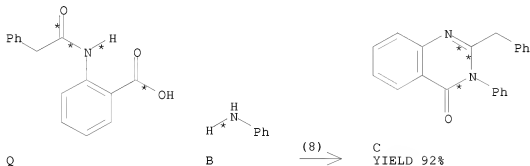
AQ
YIELD 72%

RX(21) RCT AO 2719-08-6, AP 95-53-4
RGT P 75-24-1 AlMe3
PRO AQ 72-44-6
SOL 107-06-2 ClCH2CH2Cl
CON 18 hours, reflux

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

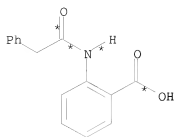
L3 ANSWER 78 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 140:321321 CASREACT
 TITLE: Eco-friendly synthesis of quinazolin-4(3H)-ones
 AUTHOR(S): Kidwai, Mazaahir; Ruby; Rastogi, Shweta
 CORPORATE SOURCE: Department of Chemistry, University of Delhi, Delhi, 110 007, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2004), 43B(2), 423-425
 CODEN: IJSBDB; ISSN: 0376-4699
 PUBLISHER: National Institute of Science Communication
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Several substituted quinazolin-4(3H)-ones were synthesized using environmentally benign procedure. Neat reactants on subjecting to microwave irradiation in the presence of dicyclohexylcarbodiimide as a condensing agent give the required products more quickly and in better yields in comparison to traditional methodologies. The observed yields and enhancement in reaction rates were due to the solvent-free conditions coupled with microwave usage.

RX(8) OF 14 Q + B ==> C

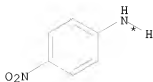


RX(8) RCT Q 28565-98-2, B 62-53-3
 RGT R 538-75-0 DCC
 PRO C 19857-34-2
 CON 2.5 minutes
 NTE microwave irradiatn., alternative preparation shown, no solvent

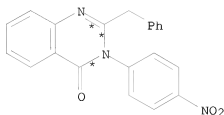
RX(9) OF 14 Q + D ==> E



Q



D



E

YIELD 93%

RX(9) RCT Q 28565-98-2, D 100-01-6
 RGT R 538-75-0 DCC
 PRO E 201293-05-2
 CON 3 minutes
 NTE microwave irradiation, alternative preparation shown, no solvent

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 79 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 140:321181 CASREACT

TITLE: First Reported Nonpeptide AT1 Receptor Agonist (L-162,313) Acts as an AT2 Receptor Agonist in Vivo
 AUTHOR(S): Wan, Yiqian; Wallinder, Charlotta; Johansson, Berndt; Holm, Mathias; Mahalingam, A. K.; Wu, Xiongyu; Botros, Milad; Karlén, Anders; Pettersson, Anders; Nyberg, Fred; Faendriks, Lars; Hallberg, Anders; Alterman, Mathias

CORPORATE SOURCE: Department of Medicinal Chemistry BMC, Uppsala University, Uppsala, SE-751 23, Swed.

SOURCE: Journal of Medicinal Chemistry (2004), 47(6), 1536-1546

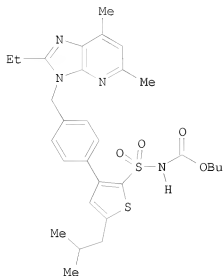
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

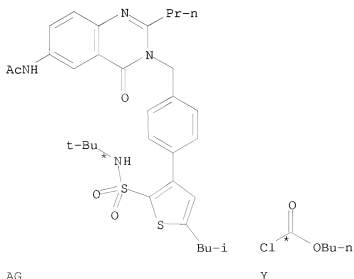
LANGUAGE: English

GI



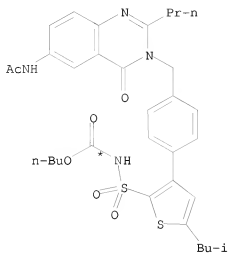
AB In this investigation, it is demonstrated that the first nonpeptide AT₁ receptor agonist L-162,313 (I), disclosed in 1994, also acts as an agonist at the AT₂ receptor. In anesthetized rats, administration of compound I i.v. or locally in the duodenum increased duodenal mucosal alkaline secretion, effects that were sensitive to the selective AT₂ receptor antagonist PD-123,319. The data strongly suggest that I is an AT₂ receptor agonist in vivo. To the best of our knowledge, this substance is the first nonpeptidic low-mol. weight compound with an agonistic effect mediated through the AT₂ receptor.

RX(11) OF 101 ...AG + Y ==> AJ



AG

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AJ
YIELD 71%

RX(11) RCT AG 678144-78-0

STAGE(1)

RGT D 100-66-3 PhOMe

SOL 76-05-1 F3CCO2H, 7732-18-5 Water

CON overnight, room temperature

STAGE(2)

RCT Y 592-34-7

RGT E 2456-81-7 4-Pyrrolidino-py

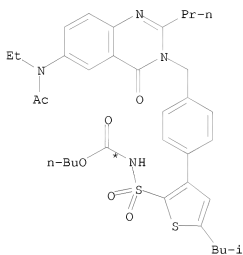
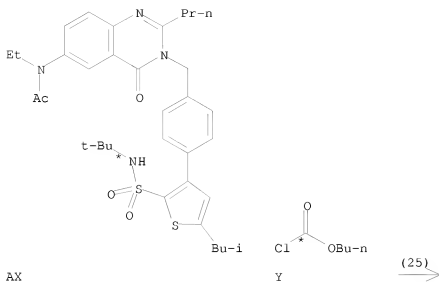
SOL 110-86-1 Pyridine

CON SUBSTAGE(1) <room temperature

SUBSTAGE(2) overnight, room temperature

PRO AJ 678144-79-1

RX(25) OF 101 ...AX + Y ==> BE



YIELD 40%

RX(25) RCT AX 678144-91-7

STAGE(1)

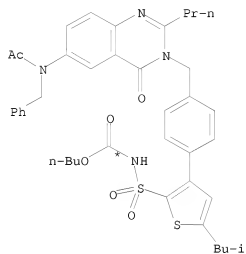
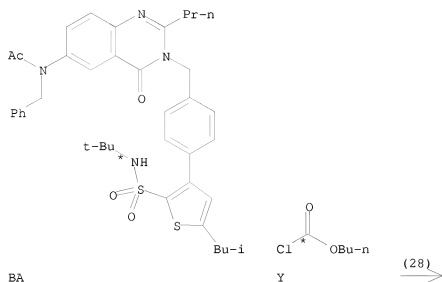
RGT D 100-66-3 PhOMe
 SOL 76-05-1 F3CCO2H, 7732-18-5 Water
 CON overnight, room temperature

STAGE(2)

RCT Y 592-34-7
 RGT E 2456-81-7 4-Pyrrolidino-py
 SOL 110-86-1 Pyridine
 CON SUBSTAGE(1) <room temperature
 SUBSTAGE(2) overnight, room temperature

PRO BE 678144-99-5

RX(28) OF 101 ...BA + Y ==> BH



YIELD 77%

RX(28) RCT BA 678144-95-1

STAGE(1)

RGT D 100-66-3 PhOMe

SOL 76-05-1 F3CCO2H, 7732-18-5 Water

CON overnight, room temperature

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STAGE(2)

RCT Y 592-34-7

RGT E 2456-81-7 4-Pyrrolidino-py

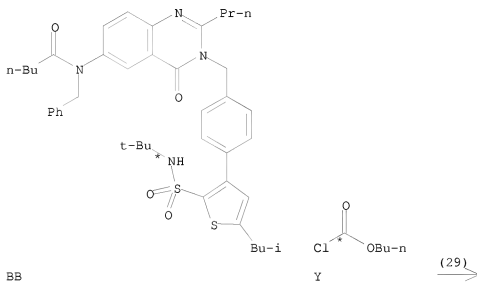
SOL 110-86-1 Pyridine

CON SUBSTAGE(1) <room temperature

SUBSTAGE(2) overnight, room temperature

PRO BH 678145-02-3

RX(29) OF 101 ...BB + Y ==> BI



BI
YIELD 68%

RX(29) RCT BB 678144-96-2

STAGE(1)

RGT D 100-66-3 PhOMe
 SOL 76-05-1 F3CCO2H, 7732-18-5 Water
 CON overnight, room temperature

STAGE(2)

RCT Y 592-34-7
 RGT E 2456-81-7 4-Pyrrolidino-py
 SOL 110-86-1 Pyridine
 CON SUBSTAGE(1) <room temperature
 SUBSTAGE(2) overnight, room temperature

PRO BI 678145-03-4

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 80 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 140:253523 CASREACT

TITLE: New 3-substituted quinazolin-4(3H)-one derivatives

AUTHOR(S): Georgescu, E.; Georgescu, Florentina; Caproiu, M. T.; Draghici, C.

CORPORATE SOURCE: "C.D. Nenitzescu" Institute of Organic Chemistry, Romanian Academy, Bucharest, Rom.

SOURCE: Scientific Bulletin - University "Politehnica" of Bucharest, Series B: Chemistry and Materials Science (2002), 64(2), 27-38

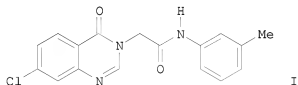
CODEN: SBUPBD; ISSN: 1454-2331

PUBLISHER: University "Politehnica" of Bucharest

DOCUMENT TYPE: Journal

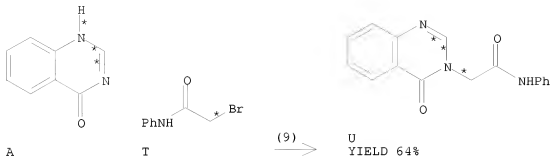
LANGUAGE: English

GI



AB 3-Substituted quinazolin-4(3H)-one derivs., e.g., I, were obtained by condensation of quinazolin-4(3H)-ones with α -halocarbonyl compds., such as α -bromo-2-acetyl thiophene and halo acetanilides, in the presence of sodium methoxide.

RX(9) OF 27 A + T ==> U



RX(9) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

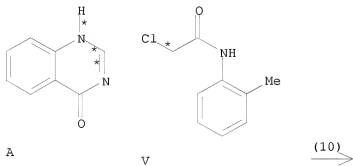
RCT T 5326-87-4

CON SUBSTAGE(1) 2 hours, reflux

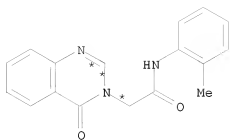
SUBSTAGE(2) overnight, cooled

PRO U 108086-38-0

RX(10) OF 27 A + V ==> W



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W
YIELD 68%

RX(10) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

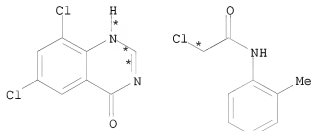
RCT V 37394-93-7

CON SUBSTAGE(1) 2 hours, reflux

SUBSTAGE(2) overnight, cooled

PRO W 374640-63-8

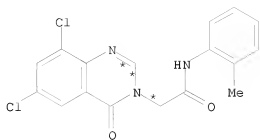
RX(12) OF 27 P + V ==> Y



P

V

(12)
→



Y
YIELD 75%

RX(12) RCT P 6952-11-0

STAGE(1)

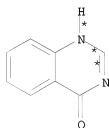
RGT D 124-41-4 NaOMe
SOL 67-56-1 MeOH
CON 10 minutes, room temperature

STAGE(2)

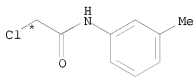
RCT V 37394-93-7
CON SUBSTAGE(1) 2 hours, reflux
SUBSTAGE(2) overnight, cooled

PRO Y 374640-80-9

RX(13) OF 27 A + Z ==> AA



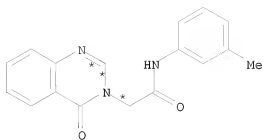
A



Z

(13) \rightarrow

10/ 562,112



AA

YIELD 71%

RX(13) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

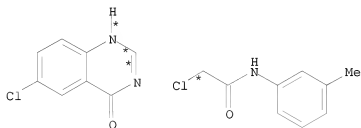
RCT Z 32428-61-8

CON SUBSTAGE(1) 2 hours, reflux

SUBSTAGE(2) overnight, cooled

PRO AA 353760-61-9

RX(14) OF 27 F + Z ==> AB

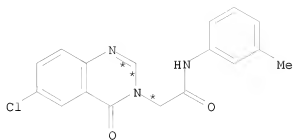


F

Z

(14)

10/ 562,112



AB

YIELD 74%

RX(14) RCT F 16064-14-5

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

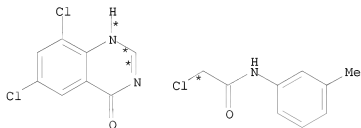
RCT Z 32428-61-8

CON SUBSTAGE(1) 2 hours, reflux

SUBSTAGE(2) overnight, cooled

PRO AB 374640-69-4

RX(16) OF 27 P + Z ==> AD

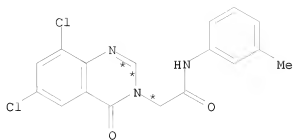


P

Z

(16)
→

10/ 562,112



AD
YIELD 73%

RX(16) RCT P 6952-11-0

STAGE(1)

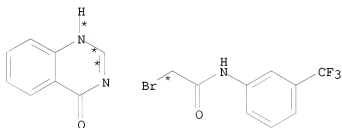
RGT D 124-41-4 NaOMe
SOL 67-56-1 MeOH
CON 10 minutes, room temperature

STAGE(2)

RCT Z 32428-61-8
CON SUBSTAGE(1) 2 hours, reflux
SUBSTAGE(2) overnight, cooled

PRO AD 374640-82-1

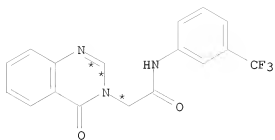
RX(17) OF 27 A + AE ==> AF



A

AE

(17) \longrightarrow



AF
YIELD 65%

RX(17) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

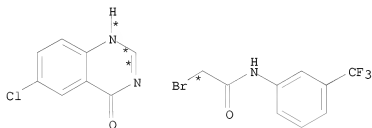
RCT AE 25625-57-4

CON SUBSTAGE(1) 2 hours, reflux

SUBSTAGE(2) overnight, cooled

PRO AF 361189-71-1

RX(18) OF 27 F + AE ==> AG

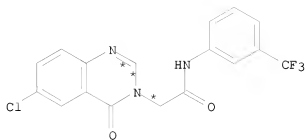


F

AE

(18) →

10/ 562,112



AG

YIELD 69%

RX(18) RCT F 16064-14-5

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

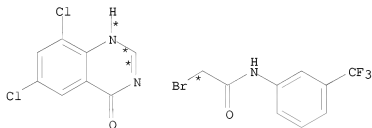
RCT AE 25625-57-4

CON SUBSTAGE(1) 2 hours, reflux

SUBSTAGE(2) overnight, cooled

PRO AG 374640-27-4

RX(20) OF 27 P + AE ==> AI

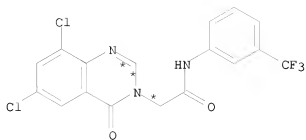


P

AE

(20)

10/ 562,112



AI
YIELD 68%

RX(20) RCT P 6952-11-0

STAGE(1)

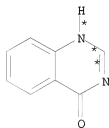
RGT D 124-41-4 NaOMe
SOL 67-56-1 MeOH
CON 10 minutes, room temperature

STAGE(2)

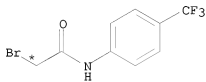
RCT AE 25625-57-4
CON SUBSTAGE(1) 2 hours, reflux
SUBSTAGE(2) overnight, cooled

PRO AI 374640-29-6

RX(21) OF 27 A + AJ ==> AK

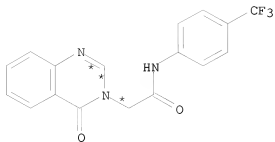


A



AJ

(21) \longrightarrow



AK

YIELD 71%

RX(21) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

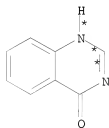
RCT AJ 3823-19-6

CON SUBSTAGE(1) 2 hours, reflux

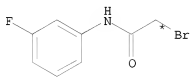
SUBSTAGE(2) overnight, cooled

PRO AK 362492-98-6

RX(22) OF 27 A + AL ==> AM



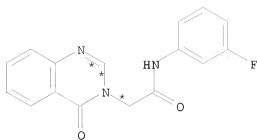
A



AL

(22)

10/ 562,112



AM

YIELD 72%

RX(22) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

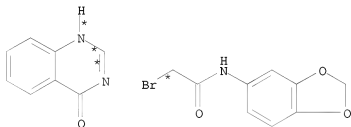
RCT AL 73392-04-8

CON SUBSTAGE(1) 2 hours, reflux

SUBSTAGE(2) overnight, cooled

PRO AM 361190-24-1

RX(23) OF 27 A + AN ==> AO

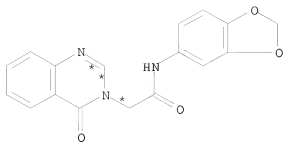


A

AN

(23)

10/ 562,112



AO

YIELD 69%

RX(23) RCT A 491-36-1

STAGE(1)

RGT D 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 10 minutes, room temperature

STAGE(2)

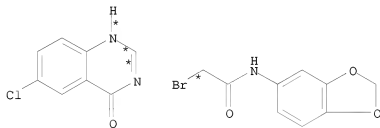
RCT AN 860806-13-9

CON SUBSTAGE(1) 2 hours, reflux

SUBSTAGE(2) overnight, cooled

PRO AO 374678-80-5

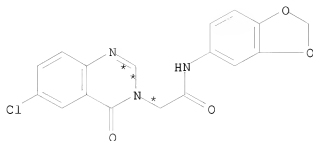
RX(24) OF 27 F + AN ==> AP



F

AN

(24) →



AP
YIELD 65%

RX(24) RCT F 16064-14-5

STAGE(1)

RGT D 124-41-4 NaOMe
SOL 67-56-1 MeOH
CON 10 minutes, room temperature

STAGE(2)

RCT AN 860806-13-9
CON SUBSTAGE(1) 2 hours, reflux
SUBSTAGE(2) overnight, cooled

PRO AP 374678-81-6

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 81 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 140:181406 CASREACT

TITLE: Amine-induced rearrangement of
4-imino-4H-3,1-benzoxazines to 4-quinazolinones via
amidine carboxamides

AUTHOR(S): Snider, Barry B.; Zeng, Hongbo
CORPORATE SOURCE: Department of Chemistry MS 015, Brandeis University,
Waltham, MA, 02454-9110, USA

SOURCE: Heterocycles (2003), 61, 173-182
CODEN: HTCYAM; ISSN: 0385-5414

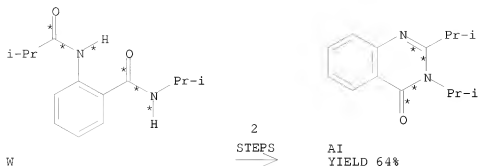
PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Iminobenzoxazines react with pyrrolidine in EtOAc at reflux to give
amidine carboxamides, which cyclize to quinazolinones on heating in 99:1
MeCN/HOAc. Some amidine intermediates could be isolated. A sterically
hindered amidine does not cyclize to give the corresponding quinazolinone.

RX(27) OF 35 COMPOSED OF RX(8), RX(20)
RX(27) W ==> AI



RX(8)

STAGE(1)

RGT G 7726-95-6 Br₂, H 603-35-0 PPh₃
 SOL 75-09-2 CH₂Cl₂
 CON 0.5 hours, room temperature

STAGE(2)

RCT W 660425-84-3
 RGT I 121-44-8 Et₃N
 CON 1.5 hours, reflux

STAGE(3)

RGT J 144-55-8 NaHCO₃
 SOL 7732-18-5 Water

PRO X 660425-89-8

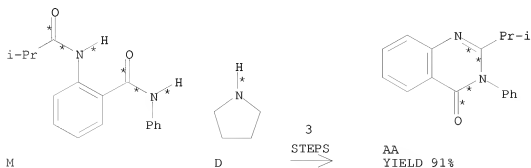
NTE mixture with 11 % of educt was isolated%

RX(20)

RCT X 660425-89-8
 RGT C 64-19-7 AcOH
 PRO AI 660425-96-7
 CAT 123-75-1 Pyrrolidine
 SOL 75-05-8 MeCN
 CON 36 hours, reflux
 NTE regioselective

RX(33) OF 35 COMPOSED OF RX(3), RX(11), RX(12)

RX(33) M + D ==> AA



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RX(3)

STAGE(1)

RGT G 7726-95-6 Br2, H 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON 0.5 hours, room temperature

STAGE(2)

RCT M 38163-55-2
RGT I 121-44-8 Et3N
CON 1.5 hours, reflux

STAGE(3)

RGT J 144-55-8 NaHCO3
SOL 7732-18-5 Water

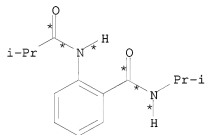
PRO N 660425-85-4

RX(11) RCT N 660425-85-4, D 123-75-1
PRO Z 660425-91-2
SOL 123-75-1 Pyrrolidine
CON 2 hours, 80 deg C
NTE alternative reaction conditions gave lower yield, alternative
reaction conditions shown

RX(12) RCT Z 660425-91-2
PRO AA 32700-64-4
CAT 64-19-7 AcOH
SOL 75-05-8 MeCN
CON 2 hours, reflux

RX(35) OF 35 COMPOSED OF RX(8), RX(17), RX(18)

RX(35) W + D ==> AI

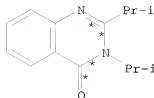


W



D

3
STEPS
→



AI
YIELD 92%

RX(8)

STAGE(1)

RGT G 7726-95-6 Br₂, H 603-35-0 PPh₃
SOL 75-09-2 CH₂Cl₂
CON 0.5 hours, room temperature

STAGE(2)

RCT W 660425-84-3
RGT I 121-44-8 Et₃N
CON 1.5 hours, reflux

STAGE(3)

RGT J 144-55-8 NaHCO₃
SOL 7732-18-5 Water

PRO X 660425-89-8
NTE mixture with 11 % of educt was isolated%

RX(17) RCT X 660425-89-8, D 123-75-1
PRO AH 660425-95-6
SOL 141-78-6 AcOEt
CON 1.5 hours, 80 deg C
NTE regioselective

RX(18) RCT AH 660425-95-6
PRO AI 660425-96-7
SOL 75-05-8 MeCN
CON 10 hours, reflux
NTE alternative reaction conditions gave lower yield, alternative reaction conditions shown

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 82 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 139:381438 CASREACT

TITLE: Various new types of macrocycles containing quinazolinone and tetrahydrobenzothienopyrimidinone rings with biological interest

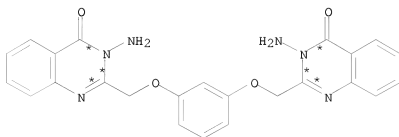
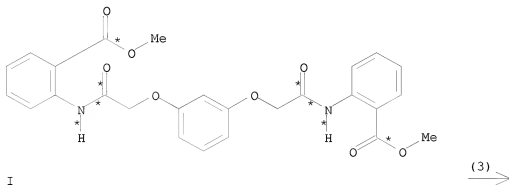
AUTHOR(S): El-Sharief, A. M. Sh.; Ammar, Y. A.; Zahran, M. A.; Ali, A. H.; El-Gaby, M. S. A.

CORPORATE SOURCE: Chemistry Department, Faculty of Science, Al-Azhar

SOURCE: University, Nasr City, Cairo, 11884, Egypt
 Afinidad (2003), 60(503), 32-41
 CODEN: AFINAE; ISSN: 0001-9704
 PUBLISHER: Asociacion de Quimicos del Instituto Quimico de Sarria
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Synthesis and characterization of new aza crown type compds. are included by reacting the corresponding bis(3-amino quinazolinone) and bis(3-aminotetrahydrobenzothieno[2,3-d]pyrimidinone) with the resp. reagents. Most of these compds. were test in vitro for their antimicrobial activities against some gram pos. and gram neg. bacteria along with their antifungal activities.

RX(3) OF 67 ...I ==> L...

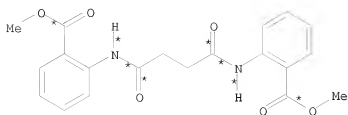


YIELD 85%

RX(3) RCT I 623928-01-8
 RGT M 302-01-2 N2H4
 PRO L 181770-29-6
 SOL 71-36-3 BuOH
 CON SUBSTAGE(1) 6 - 10 hours, reflux
 SUBSTAGE(2) reflux -> 0 deg C

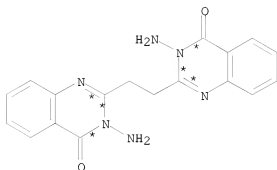
RX(13) OF 67 ...AD ==> AI...

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AD

(13) \Rightarrow

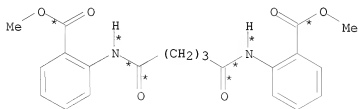


AI

YIELD 65%

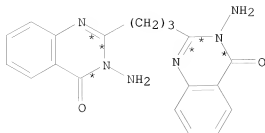
RX(13) RCT AD 501938-94-9
 RGT M 302-01-2 N₂H₄
 PRO AI 623928-08-5
 SOL 71-36-3 BuOH
 CON SUBSTAGE(1) 6 - 8 hours, reflux
 SUBSTAGE(2) reflux -> 0 deg C

RX(14) OF 67 ...AF ==> AJ...



AF

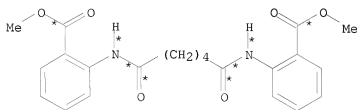
(14) \Rightarrow



AJ
YIELD 61%

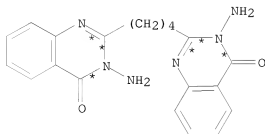
RX(14) RCT AF 352642-40-1
RGT M 302-01-2 N2H4
PRO AJ 623928-09-6
SOL 71-36-3 BuOH
CON SUBSTAGE(1) 6 - 8 hours, reflux
SUBSTAGE(2) reflux -> 0 deg C

RX(15) OF 67 ...AH ==> AK...



AH

(15) →



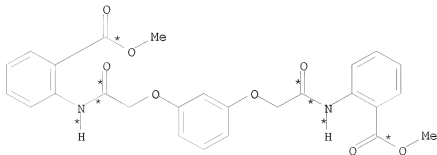
AK
YIELD 76%

RX(15) RCT AH 68191-40-2
RGT M 302-01-2 N2H4
PRO AK 623928-10-9
SOL 71-36-3 BuOH

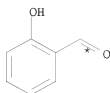
10/ 562,112

CON SUBSTAGE(1) 6 - 8 hours, reflux
SUBSTAGE(2) reflux -> 0 deg C

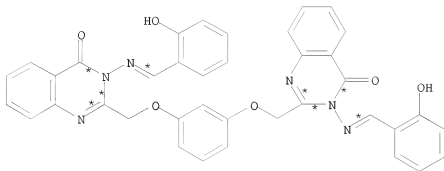
RX(28) OF 67 COMPOSED OF RX(3), RX(4)
RX(28) I + 2 O ==> P



I



2 O



P

YIELD 60%

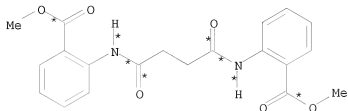
RX(3) RCT I 623928-01-8
RGT M 302-01-2 N2H4
PRO L 181770-29-6
SOL 71-36-3 BuOH
CON SUBSTAGE(1) 6 - 10 hours, reflux

10/ 562,112

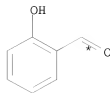
SUBSTAGE(2) reflux -> 0 deg C

RX(4) RCT L 181770-29-6, O 90-02-8
PRO P 623928-04-1
SOL 64-19-7 AcOH
CON 3 hours

RX(36) OF 67 COMPOSED OF RX(13), RX(16)
RX(36) AD + 2 O ==> AL

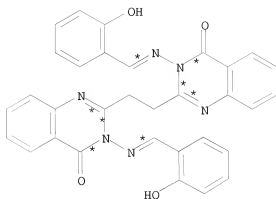


AD



2 O

2
STEPS
=>



AL
YIELD 61%

RX(13) RCT AD 501938-94-9
RGT M 302-01-2 NH4
PRO AI 623928-08-5
SOL 71-36-3 BuOH
CON SUBSTAGE(1) 6 - 8 hours, reflux
SUBSTAGE(2) reflux -> 0 deg C

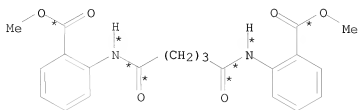
RX(16) RCT AI 623928-08-5, O 90-02-8
PRO AL 623928-11-0
SOL 64-19-7 AcOH

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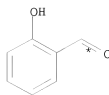
CON 1 hour, reflux

RX(38) OF 67 COMPOSED OF RX(14), RX(17)

RX(38) AF + 2 O ==> AM

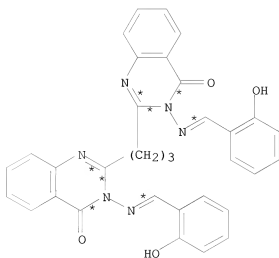


AF



2 O

2
STEPS
→



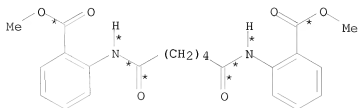
AM

YIELD 64%

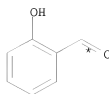
RX(14) RCT AF 352642-40-1
RGT M 302-01-2 N2H4
PRO AJ 623928-09-6
SOL 71-36-3 BuOH
CON SUBSTAGE(1) 6 - 8 hours, reflux
SUBSTAGE(2) reflux -> 0 deg C

RX(17) RCT AJ 623928-09-6, O 90-02-8
PRO AM 623928-12-1
SOL 64-19-7 AcOH
CON 1 hour, reflux

RX(40) OF 67 COMPOSED OF RX(15), RX(18)
 RX(40) AH + 2 O ==> AN

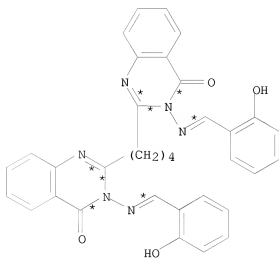


AH



2 O

2
 STEPS
 →



AN
 YIELD 60%

RX(15) RCT AH 68191-40-2
 RGT M 302-01-2 N2H4
 PRO AK 623928-10-9
 SOL 71-36-3 BuOH
 CON SUBSTAGE(1) 6 - 8 hours, reflux
 SUBSTAGE(2) reflux -> 0 deg C

RX(18) RCT AK 623928-10-9, O 90-02-8
 PRO AN 623928-13-2
 SOL 64-19-7 AcOH
 CON 1 hour, reflux

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 83 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 139:337939 CASREACT

TITLE: Yb(OTf)₃-catalyzed one-pot synthesis of quinazolin-4(3H)-ones from anthranilic acid, amines and ortho esters (or formic acid) in solvent-free conditions

AUTHOR(S): Wang, Limin; Xia, Jianjun; Qin, Fang; Qian, Changtao; Sun, Jie

CORPORATE SOURCE: Institute of Fine Chemicals, East China University of Science and Technology, Shanghai, 200237, Peop. Rep. China

SOURCE: Synthesis (2003), (8), 1241-1247

CODEN: SYNTBF; ISSN: 0039-7881

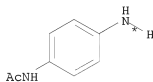
PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

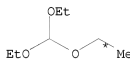
LANGUAGE: English

AB An efficient synthesis of an array of 4(3H)-quinazolinone derivs. from anthranilic acid, ortho esters (or formic acid) and amines using Yb(OTf)₃ in one-pot under solvent-free conditions is described. Compared with the classical reaction conditions, this new synthetic method has the advantage of excellent yields (75-99%), shorter reaction time (few minutes) and re-usability of the catalyst. Comps. thus prepared included 3-phenyl-4(3H)-quinazolinone, 3-(2-methylphenyl)-4(3H)-quinazolinone, 3-(4-methylphenyl)-4(3H)-quinazolinone, 3-(3,4-dimethylphenyl)-4(3H)-quinazolinone, 3-(4-ethylphenyl)-4(3H)-quinazolinone, 3-(4-methoxyphenyl)-4(3H)-quinazolinone, 3-(4-Chlorophenyl)-4(3H)-quinazolinone, 3-(4-fluorophenyl)-4(3H)-quinazolinone, 3-(4-nitrophenyl)-4(3H)-quinazolinone, etc. The lanthanide-mediated formation of an imidic ester intermediate was discussed.

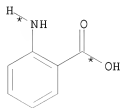
RX(22) OF 24 AO + J + A ==> AP



AO

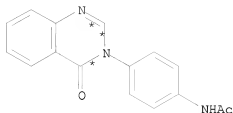


J



A

(22) →



AP
YIELD 97%

RX(22) RCT AO 122-80-5, J 122-51-0, A 118-92-3

STAGE(1)

CAT 54761-04-5 Methanesulfonic acid, 1,1,1-trifluoro-,
ytterbium(3+) salt (3:1)
CON 2 minutes, 60 deg C

STAGE(2)

SOL 7732-18-5 Water

PRO AP 24122-35-8

REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 84 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 139:181529 CASREACT

TITLE: Dyeing behaviour of some novel acid dyes on silk, wool
and nylon fabrics

AUTHOR(S): Rana, U. N.; Patel, K. C.; Patel, S. K.

CORPORATE SOURCE: Department of Chemistry, South Gujarat University,
Surat, 395 007, India

SOURCE: Ultra Scientist of Physical Sciences (2002), 14(3),
353-360

CODEN: USPSE5

PUBLISHER: Ultra Scientist of Physical Sciences

DOCUMENT TYPE: Journal

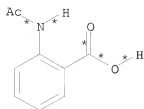
LANGUAGE: English

AB Ten azo dyes have been prepared by coupling diazotized
2-methyl-3-(2-chlorophenyl)-6-amino-4-oxoquinazoline with various coupling
acid components and their dyeing performance on silk, wool, and nylon has
been assessed. All the dyes gave a wide range of brown shades with very
good depth and levelness. The purity of all dyes has been checked by TLC.
The IR spectra showed all characteristic bands and a representative dye
PMR spectrum showed all the characteristic signals. The percentage
dye-bath exhaustion and fixation on different fibers was reasonably
moderate to very good.

RX(15) OF 60 COMPOSED OF RX(11), RX(12)

RX(15) AA + AB + AD ==> AE

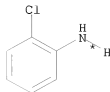
10/ 562,112



AA

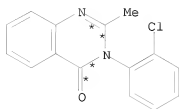


AB



AD

2
STEPS
→



AE

YIELD 85%

RX(11) RCT AA 89-52-1, AB 108-24-7
PRO AC 525-76-8
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

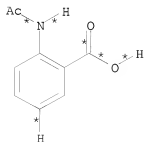
STAGE(1)
CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AE 340-57-8

RX(28) OF 60 COMPOSED OF RX(11), RX(12), RX(13)

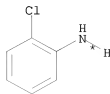
RX(28) AA + AB + AD ==> AF



AA

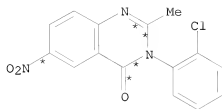


AB



AD

3
STEPS
→



AF
YIELD 90%

RX(11) RCT AA 89-52-1, AB 108-24-7
PRO AC 525-76-8
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

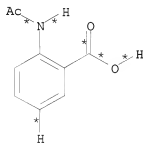
STAGE(1)
CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AE 340-57-8

RX(13) RCT AE 340-57-8
RGT AG 7697-37-2 HNO3
PRO AF 1038-70-6
SOL 7664-93-9 H2SO4
CON SUBSTAGE(1) <75 deg C
SUBSTAGE(2) overnight

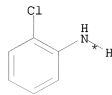
RX(30) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14)
RX(30) AA + AB + AD ==> A



AA

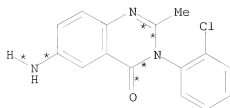


AB



AD

4
STEPS
➡



A

YIELD 85%

RX(11) RCT AA 89-52-1, AB 108-24-7
 PRO AC 525-76-8
 CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)

CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO AE 340-57-8

RX(13) RCT AE 340-57-8
 RGT AG 7697-37-2 HNO3
 PRO AF 1038-70-6
 SOL 7664-93-9 H2SO4
 CON SUBSTAGE(1) <75 deg C
 SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

STAGE(1)

RGT AI 1313-82-2 Na2S

SOL 7732-18-5 Water

CON 2 hours, reflux

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

CON 20 minutes, reflux

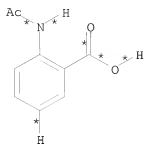
STAGE(3)

RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(51) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(1)

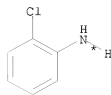
RX(51) AA + AB + AD + B ==> C



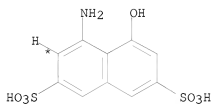
AA



AB

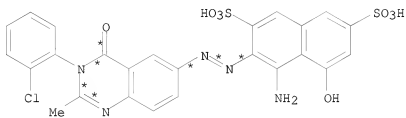


AD



B

5
STEPS
→



● 2 Na

C

YIELD 85%

RX(11) RCT AA 89-52-1, AB 108-24-7
PRO AC 525-76-8
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)

CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

```

PRO AE 340-57-8

RX(13) RCT AE 340-57-8
      RGT AG 7697-37-2 HNO3
      PRO AF 1038-70-6
      SOL 7664-93-9 H2SO4
      CON SUBSTAGE(1) <75 deg C
          SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

      STAGE(1)
      RGT AI 1313-82-2 Na2S
      SOL 7732-18-5 Water
      CON 2 hours, reflux

      STAGE(2)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON 20 minutes, reflux

      STAGE(3)
      RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(1) RCT A 963-35-9

      STAGE(1)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON SUBSTAGE(1) room temperature -> 70 deg C
          SUBSTAGE(2) 70 deg C -> 0 deg C

      STAGE(2)
      RGT E 7632-00-0 NaNO2
      SOL 7732-18-5 Water
      CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C
          SUBSTAGE(2) 1 hour, 0 - 5 deg C

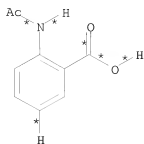
      STAGE(3)
      RGT F 5329-14-6 Sulfamic acid

      STAGE(4)
      RCT B 90-20-0
      RGT G 497-19-8 Na2CO3
      CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
          SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

PRO C 577040-28-9

RX(52) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(2)
RX(52) AA + AB + AD + I ==> J

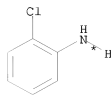
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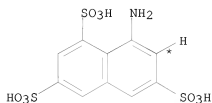
AA



AB

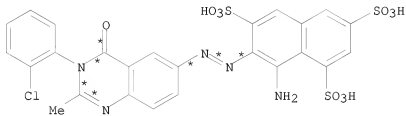


AD



I

5
STEPS
→



● 3 Na

J
YIELD 80%

RX(11) RCT AA 89-52-1, AB 108-24-7
PRO AC 525-76-8
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)
CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water


```

PRO AE 340-57-8

RX(13) RCT AE 340-57-8
      RGT AG 7697-37-2 HNO3
      PRO AF 1038-70-6
      SOL 7664-93-9 H2SO4
      CON SUBSTAGE(1) <75 deg C
          SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

      STAGE(1)
      RGT AI 1313-82-2 Na2S
      SOL 7732-18-5 Water
      CON 2 hours, reflux

      STAGE(2)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON 20 minutes, reflux

      STAGE(3)
      RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(2) RCT A 963-35-9

      STAGE(1)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON SUBSTAGE(1) room temperature -> 70 deg C
          SUBSTAGE(2) 70 deg C -> 0 deg C

      STAGE(2)
      RGT E 7632-00-0 NaNO2
      SOL 7732-18-5 Water
      CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C
          SUBSTAGE(2) 1 hour, 0 - 5 deg C

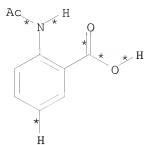
      STAGE(3)
      RGT F 5329-14-6 Sulfamic acid

      STAGE(4)
      RCT I 117-42-0
      RGT G 497-19-8 Na2CO3
      CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
          SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

PRO J 577040-29-0

RX(53) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(3)
RX(53) AA + AB + AD + K ==> L

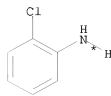
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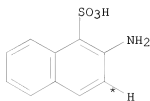
AA



AB

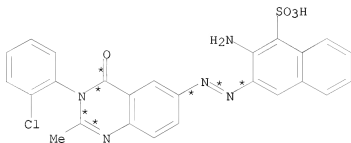


AD



K

5
STEPS
→



● Na

L
YIELD 78%

RX(11) RCT AA 89-52-1, AB 108-24-7
PRO AC 525-76-8
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)
CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)

RGT D 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AE 340-57-8

RX(13) RCT AE 340-57-8
RGT AG 7697-37-2 HNO3
PRO AF 1038-70-6
SOL 7664-93-9 H2SO4
CON SUBSTAGE(1) <75 deg C
SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

STAGE(1)
RGT AI 1313-82-2 Na2S
SOL 7732-18-5 Water
CON 2 hours, reflux

STAGE(2)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
CON 20 minutes, reflux

STAGE(3)
RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(3) RCT A 963-35-9

STAGE(1)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) room temperature -> 70 deg C
SUBSTAGE(2) 70 deg C -> 0 deg C

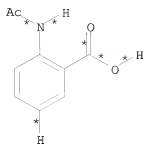
STAGE(2)
RGT E 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C
SUBSTAGE(2) 1 hour, 0 - 5 deg C

STAGE(3)
RGT F 5329-14-6 Sulfamic acid

STAGE(4)
RCT K 81-16-3
RGT G 497-19-8 Na2CO3
CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

PRO L 577040-30-3

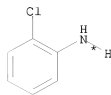
RX(54) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(4)
RX(54) AA + AB + AD + M ==> N



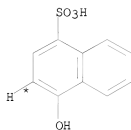
AA



AB

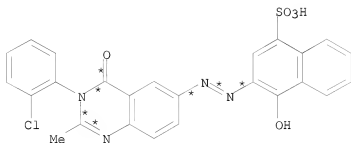


AD



M

5
STEPS
→



● Na

N
YIELD 72%

RX(11) RCT AA 89-52-1, AB 108-24-7
PRO AC 525-76-8
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)
CON 8 - 10 hours, 150 - 180 deg C

```

      STAGE(2)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water

PRO AE 340-57-8

RX(13) RCT AE 340-57-8
      RGT AG 7697-37-2 HNO3
      PRO AF 1038-70-6
      SOL 7664-93-9 H2SO4
      CON SUBSTAGE(1) <75 deg C
      SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

      STAGE(1)
      RGT AI 1313-82-2 Na2S
      SOL 7732-18-5 Water
      CON 2 hours, reflux

      STAGE(2)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON 20 minutes, reflux

      STAGE(3)
      RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(4) RCT A 963-35-9

      STAGE(1)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON SUBSTAGE(1) room temperature -> 70 deg C
      SUBSTAGE(2) 70 deg C -> 0 deg C

      STAGE(2)
      RGT E 7632-00-0 NaNO2
      SOL 7732-18-5 Water
      CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C
      SUBSTAGE(2) 1 hour, 0 - 5 deg C

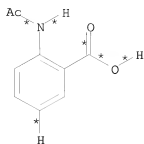
      STAGE(3)
      RGT F 5329-14-6 Sulfamic acid

      STAGE(4)
      RCT M 84-87-7
      RGT G 497-19-8 Na2CO3
      CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
      SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

PRO N 577040-31-4

RX(55) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(5)
RX(55) AA + AB + AD + O ==> P

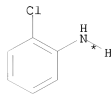
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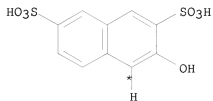
AA



AB

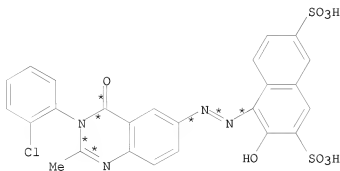


AD



O

5
STEPS
→



● 2 Na

P
YIELD 82%

RX(11) RCT AA 89-52-1, AB 108-24-7
PRO AC 525-76-8
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)
CON 8 - 10 hours, 150 - 180 deg C

```

      STAGE(2)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water

PRO AE 340-57-8

RX(13) RCT AE 340-57-8
      RGT AG 7697-37-2 HNO3
      PRO AF 1038-70-6
      SOL 7664-93-9 H2SO4
      CON SUBSTAGE(1) <75 deg C
      SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

      STAGE(1)
      RGT AI 1313-82-2 Na2S
      SOL 7732-18-5 Water
      CON 2 hours, reflux

      STAGE(2)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON 20 minutes, reflux

      STAGE(3)
      RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(5) RCT A 963-35-9

      STAGE(1)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON SUBSTAGE(1) room temperature -> 70 deg C
      SUBSTAGE(2) 70 deg C -> 0 deg C

      STAGE(2)
      RGT E 7632-00-0 NaNO2
      SOL 7732-18-5 Water
      CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C
      SUBSTAGE(2) 1 hour, 0 - 5 deg C

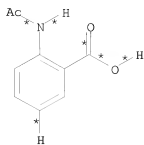
      STAGE(3)
      RGT F 5329-14-6 Sulfamic acid

      STAGE(4)
      RCT O 148-75-4
      RGT G 497-19-8 Na2CO3
      CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
      SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

PRO P 577040-32-5

RX(56) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(6)
RX(56) AA + AB + AD + Q ==> R

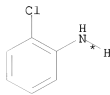
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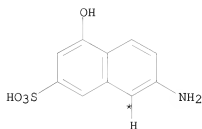
AA



AB

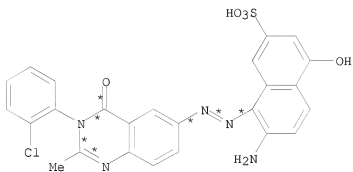


AD



Q

5
STEPS
→



● Na

R
YIELD 87%

RX(11) RCT AA 89-52-1, AB 108-24-7
PRO AC 525-76-8
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2


```

      STAGE(1)
      CON 8 - 10 hours, 150 - 180 deg C

      STAGE(2)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water

PRO AE 340-57-8

RX(13) RCT AE 340-57-8
      RGT AG 7697-37-2 HNO3
      PRO AF 1038-70-6
      SOL 7664-93-9 H2SO4
      CON SUBSTAGE(1) <75 deg C
      SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

      STAGE(1)
      RGT AI 1313-82-2 Na2S
      SOL 7732-18-5 Water
      CON 2 hours, reflux

      STAGE(2)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON 20 minutes, reflux

      STAGE(3)
      RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(6) RCT A 963-35-9

      STAGE(1)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON SUBSTAGE(1) room temperature -> 70 deg C
      SUBSTAGE(2) 70 deg C -> 0 deg C

      STAGE(2)
      RGT E 7632-00-0 NaNO2
      SOL 7732-18-5 Water
      CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C
      SUBSTAGE(2) 1 hour, 0 - 5 deg C

      STAGE(3)
      RGT F 5329-14-6 Sulfamic acid

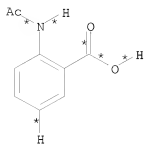
      STAGE(4)
      RCT Q 87-02-5
      RGT G 497-19-8 Na2CO3
      CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
      SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

PRO R 577040-33-6

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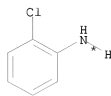
RX(57) AA + AB + AD + S ==> T



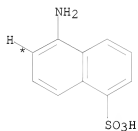
AA



AB

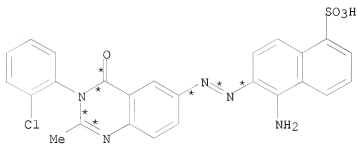


AD



S

5
STEPS
→



● Na

T
YIELD 72%

RX(11) RCT AA 89-52-1, AB 108-24-7
 PRO AC 525-76-8
 CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

```

    STAGE(1)
      CON 8 - 10 hours, 150 - 180 deg C

    STAGE(2)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water

    PRO AE 340-57-8

RX(13)  RCT AE 340-57-8
        RGT AG 7697-37-2 HNO3
        PRO AF 1038-70-6
        SOL 7664-93-9 H2SO4
        CON SUBSTAGE(1) <75 deg C
          SUBSTAGE(2) overnight

RX(14)  RCT AF 1038-70-6

    STAGE(1)
      RGT AI 1313-82-2 Na2S
      SOL 7732-18-5 Water
      CON 2 hours, reflux

    STAGE(2)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON 20 minutes, reflux

    STAGE(3)
      RGT G 497-19-8 Na2CO3

    PRO A 963-35-9

RX(7)   RCT A 963-35-9

    STAGE(1)
      RGT D 7647-01-0 HCl
      SOL 7732-18-5 Water
      CON SUBSTAGE(1) room temperature -> 70 deg C
        SUBSTAGE(2) 70 deg C -> 0 deg C

    STAGE(2)
      RGT E 7632-00-0 NaNO2
      SOL 7732-18-5 Water
      CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C
        SUBSTAGE(2) 1 hour, 0 - 5 deg C

    STAGE(3)
      RGT F 5329-14-6 Sulfamic acid

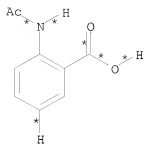
    STAGE(4)
      RCT S 84-89-9
      RGT G 497-19-8 Na2CO3
      CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
        SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

    PRO T 577040-34-7

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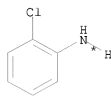
RX(58) AA + AB + AD + U ==> V



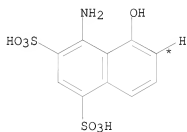
AA



AB

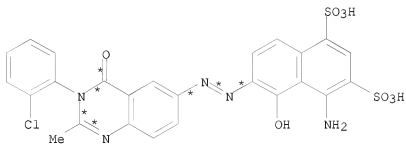


AD



U

5
STEPS
→



● 2 Na

V
YIELD 76%

RX(11) RCT AA 89-52-1, AB 108-24-7
 PRO AC 525-76-8
 CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)
CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AE 340-57-8

RX(13) RCT AE 340-57-8
RGT AG 7697-37-2 HNO3
PRO AF 1038-70-6
SOL 7664-93-9 H2SO4
CON SUBSTAGE(1) <75 deg C
SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

STAGE(1)
RGT AI 1313-82-2 Na2S
SOL 7732-18-5 Water
CON 2 hours, reflux

STAGE(2)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
CON 20 minutes, reflux

STAGE(3)
RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(8) RCT A 963-35-9

STAGE(1)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) room temperature -> 70 deg C
SUBSTAGE(2) 70 deg C -> 0 deg C

STAGE(2)
RGT E 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C
SUBSTAGE(2) 1 hour, 0 - 5 deg C

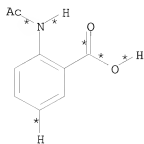
STAGE(3)
RGT F 5329-14-6 Sulfamic acid

STAGE(4)
RCT U 82-47-3
RGT G 497-19-8 Na2CO3
CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

PRO V 577040-35-8

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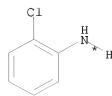
RX(59) AA + AB + AD + W ==> X



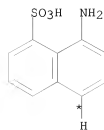
AA



AB

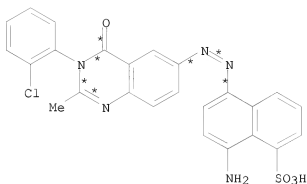


AD



W

5
STEPS
→



● Na

X
YIELD 79%

RX(11) RCT AA 89-52-1, AB 108-24-7
 PRO AC 525-76-8
 CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)
CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water

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PRO AE 340-57-8

RX(13) RCT AE 340-57-8
RGT AG 7697-37-2 HNO3
PRO AF 1038-70-6
SOL 7664-93-9 H2SO4
CON SUBSTAGE(1) <75 deg C
SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

STAGE(1)
RGT AI 1313-82-2 Na2S
SOL 7732-18-5 Water
CON 2 hours, reflux

STAGE(2)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
CON 20 minutes, reflux

STAGE(3)
RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(9) RCT A 963-35-9

STAGE(1)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) room temperature -> 70 deg C
SUBSTAGE(2) 70 deg C -> 0 deg C

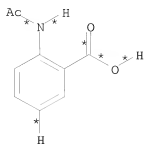
STAGE(2)
RGT E 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C
SUBSTAGE(2) 1 hour, 0 - 5 deg C

STAGE(3)
RGT F 5329-14-6 Sulfamic acid

STAGE(4)
RCT W 82-75-7
RGT G 497-19-8 Na2CO3
CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

PRO X 577040-36-9

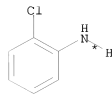
RX(60) OF 60 COMPOSED OF RX(11), RX(12), RX(13), RX(14), RX(10)
RX(60) AA + AB + AD + Y ==> Z



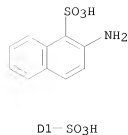
AA



AB

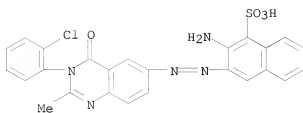


AD



Y

5
STEPS
→

D1-SO₃H

● 2 Na

Z
YIELD 82%

RX(11) RCT AA 89-52-1, AB 108-24-7
PRO AC 525-76-8
CON 30 minutes, reflux

RX(12) RCT AC 525-76-8, AD 95-51-2

STAGE(1)
CON 8 - 10 hours, 150 - 180 deg C

STAGE(2)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AE 340-57-8

RX(13) RCT AE 340-57-8
RGT AG 7697-37-2 HNO₃

PRO AF 1038-70-6
SOL 7664-93-9 H2SO4
CON SUBSTAGE(1) <75 deg C
SUBSTAGE(2) overnight

RX(14) RCT AF 1038-70-6

STAGE(1)
RGT AI 1313-82-2 Na2S
SOL 7732-18-5 Water
CON 2 hours, reflux

STAGE(2)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
CON 20 minutes, reflux

STAGE(3)
RGT G 497-19-8 Na2CO3

PRO A 963-35-9

RX(10) RCT A 963-35-9

STAGE(1)
RGT D 7647-01-0 HCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) room temperature -> 70 deg C
SUBSTAGE(2) 70 deg C -> 0 deg C

STAGE(2)
RGT E 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON SUBSTAGE(1) 5 minutes, 0 - 5 deg C
SUBSTAGE(2) 1 hour, 0 - 5 deg C

STAGE(3)
RGT F 5329-14-6 Sulfamic acid

STAGE(4)
RCT Y 171570-11-9
RGT G 497-19-8 Na2CO3
CON SUBSTAGE(1) 10 - 15 minutes, 0 deg C, pH 7.5 - 8
SUBSTAGE(2) 3 hours, <5 deg C, pH 7.5 - 8

PRO Z 577969-58-5

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 85 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 139:101143 CASREACT
TITLE: Preparation of quinazolinone derivatives having
poly(adenosine 5'-diphosphoribose) polymerase
inhibitory activity

INVENTOR(S): Ishida, Junya; Hattori, Kouji; Kido, Yoshiyuki
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 35 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

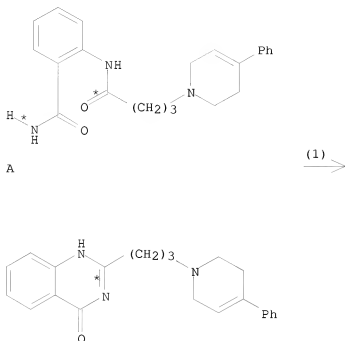
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003055865	A1	20030710	WO 2002-JP13286	20021219
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, BG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2471348	A1	20030710	CA 2002-2471348	20021219
AU 2002353537	A1	20030715	AU 2002-353537	20021219
EP 1458688	A1	20040922	EP 2002-788856	20021219
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
JP 200515216	T	20050526	JP 2003-556396	20021219
US 20050043333	A1	20050224	US 2004-499348	20040617
PRIORITY APPLN. INFO.:			AU 2001-9756	20011224
			WO 2002-JP13286	20021219
OTHER SOURCE(S):	MARPAT 139:101143			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Quinazolinone derivs. I [R1 = substituted cyclic amino, (un)substituted amino; R2 = substituent - halogen, lower alkyl, lower alkoxy; n = integer from 0 to 4; L1 = (1) cyclo (lower) alkylenes, (2) cyclo (lower) alkenylene, (3) diradical of (un)saturated monocyclic group with one or more nitrogen atom(s), which is obtained after removal of one hydrogen atom from said monocyclic group, or (4) -N(R3)-L2-; R3 = H, lower alkyl; L2 = lower alkylenes or lower alkenylene], or its prodrug, or a salt thereof having poly(adenosine 5'-diphospho-ribose) polymerase (PARP) inhibitory activity and their preparation from benzamides II are described. Thus, III was prepared via cyclization of benzamide IV in dioxane with aqueous NaOH. PARP inhibitory activity of I [] was determined (IC50 = <0.5 μ M).

RX(1) OF 5 A ==> B

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B
YIELD 70%

RX(1) RCT A 437998-41-9

STAGE(1)
SOL 123-91-1 Dioxane
CON room temperature

STAGE(2)
RGT C 1310-73-2 NaOH
SOL 7732-18-5 Water
CON 15 hours, room temperature

PRO B 437995-37-4
NTE key step

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 86 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 139:69214 CASREACT
TITLE: Improved synthesis of
3-(2-ethylphenyl)-2-methyl-4(3H)-quinazolinone
hydrochloride
AUTHOR(S): Yu, Hong-Xia; Guo, Feng; Xu, Xiong-li
CORPORATE SOURCE: Department Pharmacy, Wuhan Inst. Chem. Technol.,
Wuhan, 430073, Peop. Rep. China
SOURCE: Wuhan Huagong Xueyuan Xuebao (2002), 24(4), 13-14

CODEN: WXUXEY; ISSN: 1004-4736

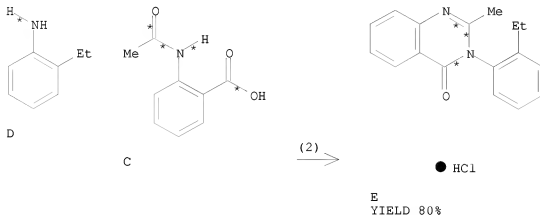
PUBLISHER: Wuhan Huagong Xueyuan Xuebao Bianjibu

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB Refluxing 2-acetylaminobenzoic acid with 2-ethylaniline in toluene in the presence of POCl₃ for 3 h gave 80% the title compound

RX(2) OF 3 ...D + C ==> E



RX(2) RCT D 578-54-1, C 89-52-1
RGT F 10025-87-3 POCl₃
PRO E 97979-65-2
SOL 108-88-3 PhMe
CON 3 hours, reflux

L3 ANSWER 87 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 139:22171 CASREACT

TITLE: Synthesis of some new substituted
β-(quinazolin-2-yl) acrylic acid derivatives of
expected biological activity

AUTHOR(S): Nassar, S. A.; Aly, A. A.

CORPORATE SOURCE: Chemistry Department, Faculty of Science, Benha
Branch, Zagazig University, Benha, Egypt

SOURCE: Egyptian Journal of Chemistry (2002), 45(1), 205-217
CODEN: EGJCA3; ISSN: 0449-2285

PUBLISHER: National Information and Documentation Centre

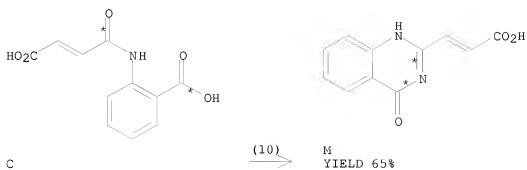
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Some new substituted β-(quinazolin-2-yl) acrylic acid derivs. were synthesized from the reaction of 2-(2'-carboxyethenyl)-4H-3,1-benzoxazin-4-one with nitrogen nucleophiles. The structures of the synthesized compds. were confirmed by IR, NMR, and mass spectral study. The products were screened for their antimicrobial activity. Most of the compds. exhibited moderate activity.

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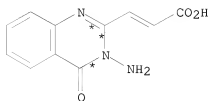
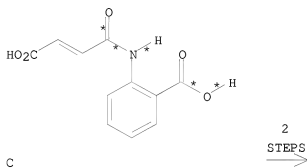
RX(10) OF 101 ...C ==> M...



RX(10) RCT C 68040-76-6
 RGT Z 631-61-8 NH4OAc
 PRO M 5584-96-3
 CON 1 hour, 170 deg C

RX(38) OF 101 COMPOSED OF RX(2), RX(3)

RX(38) C ==> E



E
YIELD 70%

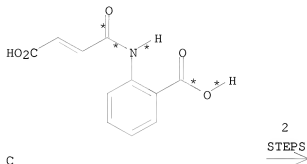
RX(2) RCT C 68040-76-6
 PRO D 107855-44-7
 CON 1 hour

RX(3) RCT D 107855-44-7

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RGT F 7803-57-8 N2H4-H2O
PRO E 536741-94-3
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(39) OF 101 COMPOSED OF RX(2), RX(4)
RX(39) C ==> H



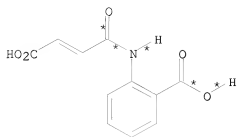
H
YIELD 75%

RX(2) RCT C 68040-76-6
PRO D 107855-44-7
CON 1 hour

RX(4) RCT D 107855-44-7
RGT I 5470-11-1 H2NOH-HCl, J 110-86-1 Pyridine
PRO H 37833-86-6
CON 4 hours, reflux

RX(40) OF 101 COMPOSED OF RX(2), RX(5)
RX(40) C + K ==> L

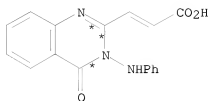
10/ 562,112



C



2
STEPS
➤

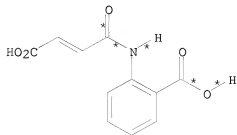


L
YIELD 68%

RX(2) RCT C 68040-76-6
PRO D 107855-44-7
CON 1 hour

RX(5) RCT D 107855-44-7, K 100-63-0
RGT F 7803-57-8 N2H4-H2O
PRO L 5958-13-4
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(41) OF 101 COMPOSED OF RX(2), RX(16)
RX(41) C + AJ ==> AK

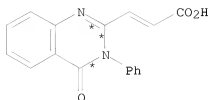


C



2
STEPS
➤

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AK

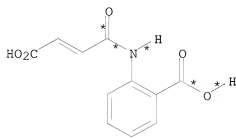
YIELD 74%

RX(2) RCT C 68040-76-6
PRO D 107855-44-7
CON 1 hour

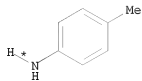
RX(16) RCT D 107855-44-7, AJ 62-53-3
PRO AK 536742-04-8
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(42) OF 101 COMPOSED OF RX(2), RX(17)

RX(42) C + AL ==> AM

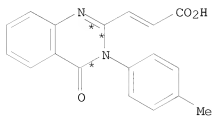


C



AL

2
STEPS
→



AM

YIELD 70%

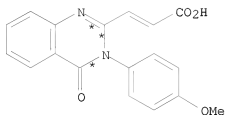
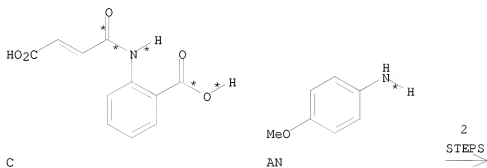
RX(2) RCT C 68040-76-6
PRO D 107855-44-7

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CON 1 hour

RX(17) RCT D 107855-44-7, AL 106-49-0
PRO AM 536742-05-9
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(43) OF 101 COMPOSED OF RX(2), RX(18)
RX(43) C + AN ==> AO



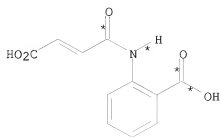
AO
YIELD 68%

RX(2) RCT C 68040-76-6
PRO D 107855-44-7
CON 1 hour

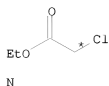
RX(18) RCT D 107855-44-7, AN 104-94-9
PRO AO 536742-06-0
SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(54) OF 101 COMPOSED OF RX(10), RX(6)
RX(54) C + N ==> O

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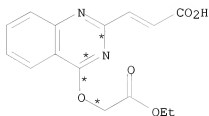


C



N

2
STEPS
→



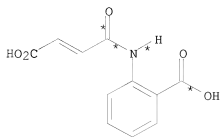
O

YIELD 62%

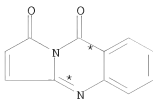
RX(10) RCT C 68040-76-6
RGT Z 631-61-8 NH4OAc
PRO M 5584-96-3
CON 1 hour, 170 deg C

RX(6) RCT M 5584-96-3, N 105-39-5
RGT P 584-08-7 K2CO3
PRO O 536741-95-4
SOL 67-64-1 Me2CO
CON 24 hours

RX(55) OF 101 COMPOSED OF RX(10), RX(11)
RX(55) C + AA ==> L



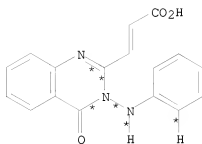
C



AA

2
STEPS
→

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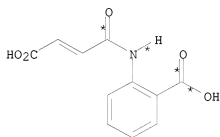


L
YIELD 65%

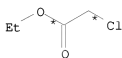
RX(10) RCT C 68040-76-6
RGT Z 631-61-8 NH4OAc
PRO M 5584-96-3
CON 1 hour, 170 deg C

RX(11) RCT AA 536741-99-8, M 5584-96-3
RGT AB 64-19-7 AcOH
PRO L 5958-13-4
SOL 64-19-7 AcOH
CON SUBSTAGE(1) 80 deg C
SUBSTAGE(2) 1 hour, 140 - 150 deg C
NTE polyphosphoric acid

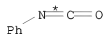
RX(74) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(9)
RX(74) C + N + X ==> Y



C

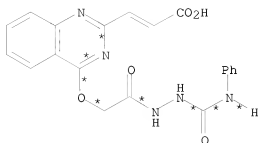


N



X

4
STEPS
→



Y
YIELD 63%

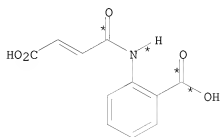
RX(10) RCT C 68040-76-6
RGT Z 631-61-8 NH4OAc
PRO M 5584-96-3
CON 1 hour, 170 deg C

RX(6) RCT M 5584-96-3, N 105-39-5
RGT P 584-08-7 K2CO3
PRO O 536741-95-4
SOL 67-64-1 Me2CO
CON 24 hours

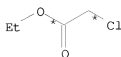
RX(8) RCT O 536741-95-4
RGT W 302-01-2 N2H4
PRO V 536741-97-6
SOL 64-17-5 EtOH
CON 3 hours, reflux

RX(9) RCT V 536741-97-6, X 103-71-9
PRO Y 536741-98-7
SOL 64-17-5 EtOH
CON 4 hours, reflux

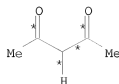
RX(75) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(12)
RX(75) C + N + AC ==> AD



C

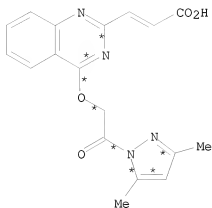


N



AC

4
STEPS
→



AD
YIELD 59%

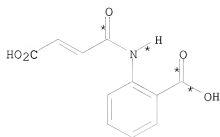
RX(10) RCT C 68040-76-6
RGT Z 631-61-8 NH4OAc
PRO M 5584-96-3
CON 1 hour, 170 deg C

RX(6) RCT M 5584-96-3, N 105-39-5
RGT P 584-08-7 K2CO3
PRO O 536741-95-4
SOL 67-64-1 Me2CO
CON 24 hours

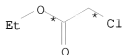
RX(8) RCT O 536741-95-4
RGT W 302-01-2 N2H4
PRO V 536741-97-6
SOL 64-17-5 EtOH
CON 3 hours, reflux

RX(12) RCT AC 123-54-6, V 536741-97-6
PRO AD 536742-00-4
SOL 64-17-5 EtOH
CON 4 hours, reflux

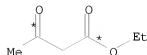
RX(76) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(13)
RX(76) C + N + AE ==> AF



C

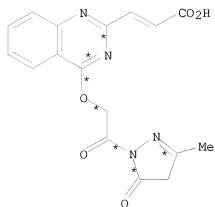


N



AE

4
STEPS
→

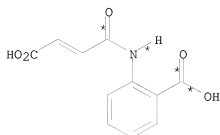


AF
YIELD 60%

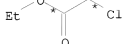
RX(10)	RCT	C 68040-76-6
	RGT	Z 631-61-8 NH4OAc
	PRO	M 5584-96-3
	CON	1 hour, 170 deg C
RX(6)	RCT	M 5584-96-3, N 105-39-5
	RGT	P 584-08-7 K2CO3
	PRO	O 536741-95-4
	SOL	67-64-1 Me2CO
	CON	24 hours
RX(8)	RCT	O 536741-95-4
	RGT	W 302-01-2 N2H4
	PRO	V 536741-97-6
	SOL	64-17-5 EtOH
	CON	3 hours, reflux
RX(13)	RCT	AE 141-97-9, V 536741-97-6
	PRO	AF 536742-01-5
	SOL	64-17-5 EtOH
	CON	4 hours, reflux

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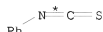
RX(77) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(15)
 RX(77) C + N + AH ==> AI



C

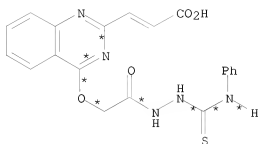


N



AH

4
 STEPS
 →



AI
 YIELD 60%

RX(10) RCT C 68040-76-6
 RGT Z 631-61-8 NH4OAc
 PRO M 5584-96-3
 CON 1 hour, 170 deg C

RX(6) RCT M 5584-96-3, N 105-39-5
 RGT P 584-08-7 K2CO3
 PRO O 536741-95-4
 SOL 67-64-1 Me2CO
 CON 24 hours

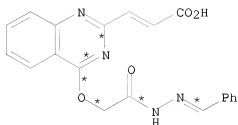
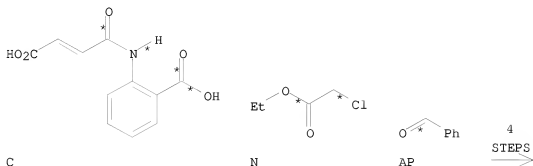
RX(8) RCT O 536741-95-4
 RGT W 302-01-2 N2H4
 PRO V 536741-97-6
 SOL 64-17-5 EtOH
 CON 3 hours, reflux

RX(15) RCT V 536741-97-6, AH 103-72-0
 PRO AI 536742-03-7

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SOL 64-17-5 EtOH
CON 4 hours, reflux

RX(78) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(19)
RX(78) C + N + AP ==> AQ



AQ
YIELD 60%

RX(10) RCT C 68040-76-6
RGT Z 631-61-8 NH4OAc
PRO M 5584-96-3
CON 1 hour, 170 deg C

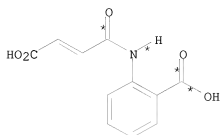
RX(6) RCT M 5584-96-3, N 105-39-5
RGT P 584-08-7 K2CO3
PRO O 536741-95-4
SOL 67-64-1 Me2CO
CON 24 hours

RX(8) RCT O 536741-95-4
RGT W 302-01-2 N2H4
PRO V 536741-97-6
SOL 64-17-5 EtOH
CON 3 hours, reflux

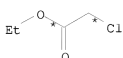
RX(19) RCT V 536741-97-6, AP 100-52-7
PRO AQ 536742-07-1
SOL 64-17-5 EtOH
CON 3 hours, reflux

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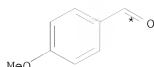
RX(79) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(20)
 RX(79) C + N + AR ==> AS



C

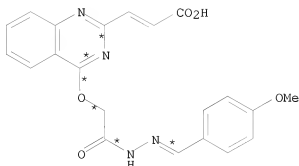


N



AR

4
 STEPS
 →



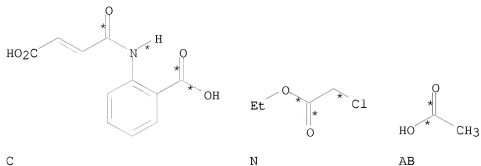
AS
 YIELD 65%

RX(10)	RCT	C 68040-76-6
	RGT	Z 631-61-8 NH4OAc
	PRO	M 5584-96-3
	CON	1 hour, 170 deg C
RX(6)	RCT	M 5584-96-3, N 105-39-5
	RGT	P 584-08-7 K2CO3
	PRO	O 536741-95-4
	SOL	67-64-1 Me2CO
	CON	24 hours
RX(8)	RCT	O 536741-95-4
	RGT	W 302-01-2 N2H4
	PRO	V 536741-97-6
	SOL	64-17-5 EtOH
	CON	3 hours, reflux

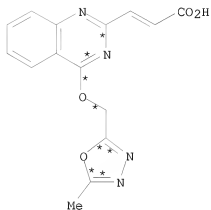
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RX(20) RCT V 536741-97-6, AR 123-11-5
 PRO AS 536742-08-2
 SOL 64-17-5 EtOH
 CON 3 hours, reflux

RX(80) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(23)
 RX(80) C + N + AB ==> AW



4
 STEPS
 →



AW
 YIELD 70%

RX(10) RCT C 68040-76-6
 RGT Z 631-61-8 NH4OAc
 PRO M 5584-96-3
 CON 1 hour, 170 deg C

RX(6) RCT M 5584-96-3, N 105-39-5
 RGT P 584-08-7 K2CO3
 PRO O 536741-95-4
 SOL 67-64-1 Me2CO
 CON 24 hours

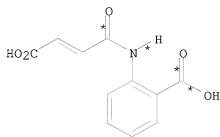
RX(8) RCT O 536741-95-4
 RGT W 302-01-2 N2H4
 PRO V 536741-97-6

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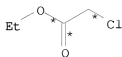
SOL 64-17-5 EtOH
CON 3 hours, reflux

RX(23) RCT AB 64-19-7, V 536741-97-6
RGT AX 10025-87-3 POC13
PRO AW 536742-11-7
SOL 64-17-5 EtOH
CON 5 hours, reflux

RX(81) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(24)
RX(81) C + N + AY ==> AZ



C

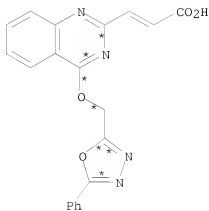


N



AY

4
STEPS
=>

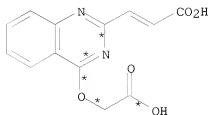
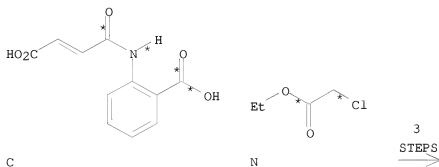


AZ
YIELD 71%

RX(10) RCT C 68040-76-6
RGT Z 631-61-8 NH4OAc
PRO M 5584-96-3
CON 1 hour, 170 deg C

RX (6)	RCT	M 5584-96-3, N 105-39-5
	RGT	P 584-08-7 K2CO3
	PRO	O 536741-95-4
	SOL	67-64-1 Me2CO
	CON	24 hours
RX (8)	RCT	O 536741-95-4
	RGT	W 302-01-2 N2H4
	PRO	V 536741-97-6
	SOL	64-17-5 EtOH
	CON	3 hours, reflux
RX (24)	RCT	AY 65-85-0, V 536741-97-6
	RGT	AX 10025-87-3 POC13
	PRO	AZ 536742-12-8
	SOL	64-17-5 EtOH
	CON	5 hours, reflux

RX(86) OF 101 COMPOSED OF RX(10), RX(6), RX(7)
 RX(86) C + N ==> R



R
YIELD 70%

RX(10)	RCT	C 68040-76-6
	RGT	Z 631-61-8 NH40Ac
	PRO	M 5584-96-3
	CON	1 hour, 170 deg C
RX(6)	RCT	M 5584-96-3, N 105-39-5
	RGT	P 584-08-7 K2CO3

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PRO O 536741-95-4
SOL 67-64-1 Me2CO
CON 24 hours

RX(7) RCT O 536741-95-4

STAGE(1)

RGT S 1310-73-2 NaOH
SOL 7732-18-5 Water
CON 3 hours, reflux

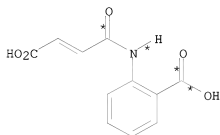
STAGE(2)

RGT T 7647-01-0 HCl
SOL 7732-18-5 Water

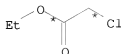
PRO R 536741-96-5

RX(87) OF 101 COMPOSED OF RX(10), RX(6), RX(8)

RX(87) C + N ==> V

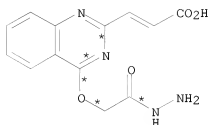


C



N

3
STEPS
→



V

YIELD 67%

RX(10) RCT C 68040-76-6
RGT Z 631-61-8 NH4OAc
PRO M 5584-96-3
CON 1 hour, 170 deg C

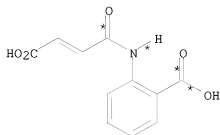
RX(6) RCT M 5584-96-3, N 105-39-5
RGT P 584-08-7 K2CO3
PRO O 536741-95-4

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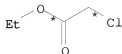
SOL 67-64-1 Me2CO
CON 24 hours

RX(8) RCT O 536741-95-4
RGT W 302-01-2 N2H4
PRO V 536741-97-6
SOL 64-17-5 EtOH
CON 3 hours, reflux

RX(98) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(19), RX(21)
RX(98) C + N + AP + AT ==> AU



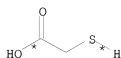
C



N

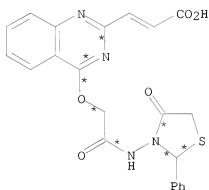


AP



AT

5
STEPS
→



AU
YIELD 61%

RX(10) RCT C 68040-76-6
RGT Z 631-61-8 NH4OAc
PRO M 5584-96-3
CON 1 hour, 170 deg C

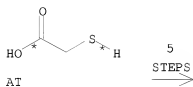
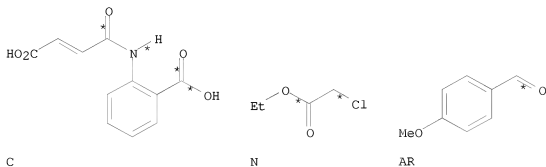
RX(6) RCT M 5584-96-3, N 105-39-5
 RGT P 584-08-7 K2CO3
 PRO O 536741-95-4
 SOL 67-64-1 Me2CO
 CON 24 hours

 RX(8) RCT O 536741-95-4
 RGT W 302-01-2 N2H4
 PRO V 536741-97-6
 SOL 64-17-5 EtOH
 CON 3 hours, reflux

 RX(19) RCT V 536741-97-6, AP 100-52-7
 PRO AQ 536742-07-1
 SOL 64-17-5 EtOH
 CON 3 hours, reflux

 RX(21) RCT AQ 536742-07-1, AT 68-11-1
 PRO AU 536742-09-3
 SOL 64-17-5 EtOH
 CON 3 hours, reflux

RX(99) OF 101 COMPOSED OF RX(10), RX(6), RX(8), RX(20), RX(22)
 RX(99) C + N + AR + AT ==> AV



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(10) RCT C 68040-76-6
 RGT Z 631-61-8 NH4OAc
 PRO M 5584-96-3
 CON 1 hour, 170 deg C

 RX(6) RCT M 5584-96-3, N 105-39-5

RGT P 584-08-7 K2CO3
 PRO O 536741-95-4
 SOL 67-64-1 Me2CO
 CON 24 hours

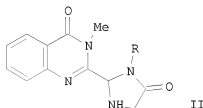
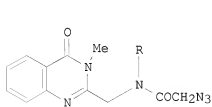
 RX(8) RCT O 536741-95-4
 RGT W 302-01-2 N2H4
 PRO V 536741-97-6
 SOL 64-17-5 EtOH
 CON 3 hours, reflux

 RX(20) RCT V 536741-97-6, AR 123-11-5
 PRO AS 536742-08-2
 SOL 64-17-5 EtOH
 CON 3 hours, reflux

 RX(22) RCT AS 536742-08-2, AT 68-11-1
 PRO AV 536742-10-6
 SOL 64-17-5 EtOH
 CON 3 hours, reflux

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

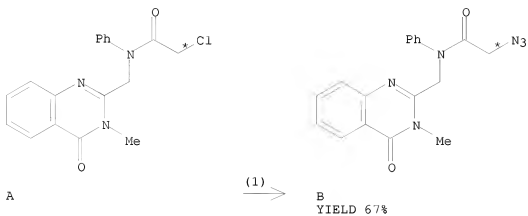
L3 ANSWER 88 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 139:6837 CASREACT
 TITLE: Synthesis of 2-quinazolinonyl imidazolidinones
 AUTHOR(S): Reddy, P. S. N.; Reddy, P. Pratap; Vasantha, T.
 CORPORATE SOURCE: Dep. of Chem., Osmania Univ., Hyderabad, 500 007, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2003), 42B(2), 393-396
 CODEN: IJSBDB; ISSN: 0376-4699
 PUBLISHER: National Institute of Science Communication
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB 2-Chloromethyl-3-methylquinazolin-4(3H)-one is converted to azides I (R = Ph, substituted Ph) which easily undergoes cyclization to give 2-quinazolinonyl imidazolidinones II. I (R = p-MeC6H4), however, yield 2,3-dimethylquinazolin-4(3H)-one and/or 2-(p-tolylaminomethyl)-3-methylquinazolin-4(3H)-one under thermal, microwave and in acidic medium.

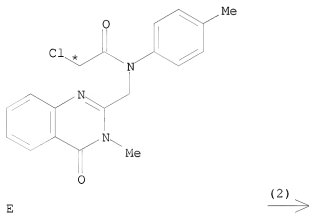
10/ 562,112

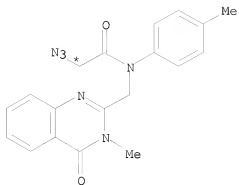
RX(1) OF 15 A ==> B...



RX(1) RCT A 228871-37-2
 RGT C 26628-22-8 NaN₃
 PRO B 536697-61-7
 SOL 68-12-2 DMF
 CON 1 hour, room temperature

RX(2) OF 15 E ==> F...

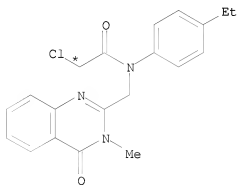




F
YIELD 80%

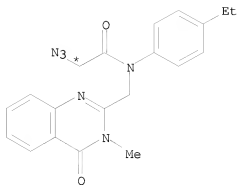
RX(2) RCT E 228871-38-3
 RGT C 26628-22-8 NaN3
 PRO F 536697-62-8
 SOL 68-12-2 DMF
 CON 1 hour, room temperature

RX(3) OF 15 G ==> H...



G

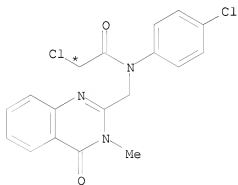
(3) →



H
YIELD 79%

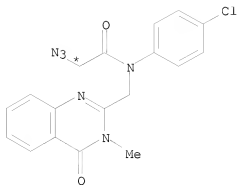
RX(3) RCT G 228871-40-7
 RGT C 26628-22-8 NaN3
 PRO H 536697-63-9
 SOL 68-12-2 DMF
 CON 1 hour, room temperature

RX(4) OF 15 I ==> J...



I

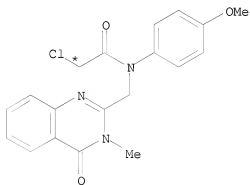
(4) →



J
YIELD 90%

RX(4) RCT I 228871-41-8
 RGT C 26628-22-8 NaN3
 PRO J 536697-64-0
 SOL 68-12-2 DMF
 CON 1 hour, room temperature

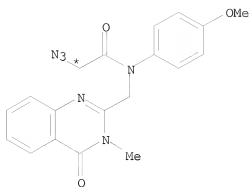
RX(5) OF 15 K ==> L



K

(5) →

10/ 562,112

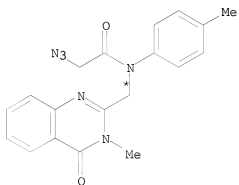


L

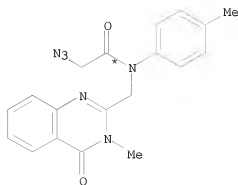
YIELD 72%

RX(5) RCT K 228871-39-4
 RGT C 26628-22-8 NaN₃
 PRO L 536697-65-1
 SOL 68-12-2 DMF
 CON 1 hour, room temperature

RX(10) OF 15 ...2 F ==> S + T

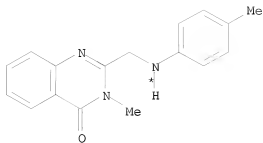


F

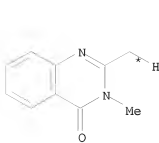


F

(10) →



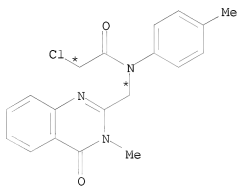
S
YIELD 20%



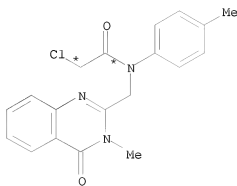
T
YIELD 50%

RX(10) RCT F 536697-62-8
RGT U 1493-13-6 F3CSO2H
PRO S 228871-31-6, T 1769-25-1
SOL 75-09-2 CH2Cl2
CON 40 hours, room temperature

RX(13) OF 15 COMPOSED OF RX(2), RX(10)
RX(13) 2 E ==> S + T

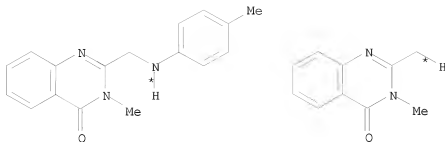


E



E

2
STEPS
→



S
YIELD 20%

T
YIELD 50%

RX(2) RCT E 228871-38-3
RGT C 26628-22-8 NaN3
PRO F 536697-62-8
SOL 68-12-2 DMF
CON 1 hour, room temperature

RX(10) RCT F 536697-62-8
RGT U 1493-13-6 F3CSO2H
PRO S 228871-31-6, T 1769-25-1
SOL 75-09-2 CH2Cl2
CON 40 hours, room temperature

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 89 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 138:338095 CASREACT

TITLE: Di-6R,7R1-4(3H)-oxo-2-quinazolinyl-substituted

cyclobutanes from pinic and sym-homopinic acids

Avotin'sh, F.; Petrova, M.; Strakovs, A.

Riga Technical University, Riga, LV-1658, Latvia

Chemistry of Heterocyclic Compounds (New York, NY,

United States)(Translation of Khimiya

Geterotsiklicheskikh Soedinenii) (2002), 38(7),

817-821

CODEN: CHCCAL; ISSN: 0009-3122

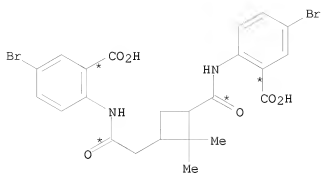
PUBLISHER: Kluwer Academic/Consultants Bureau

DOCUMENT TYPE: Journal

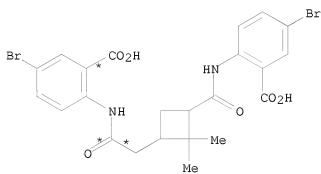
LANGUAGE: English

AB Diamides were obtained by reaction of
cis-3-carboxy-2,2-dimethylcyclobutylacetic acid (pinic acid) and of
cis/trans-3-(carboxymethyl)-2,2-dimethylcyclobutylacetic acid (homopinic
acid) dichlorides with two equivalent of 5-bromo-, 4-chloro-, and
4,5-dimethoxyanthranilic acids. Treatment of the diamides with formamide
leads to 2,2-dimethyl-3-[4(3H)-oxo-2-quinazolinyl]methyl-1-[4(3H)-oxo-2-
quinazolinyl]cyclobutanes and 2,2-dimethyl-1,3-di[4(3H)-oxo-2-
quinazolinylmethyl]cyclobutanes.

RX(7) OF 18 ...2 C + 3 N ==> O + P



C

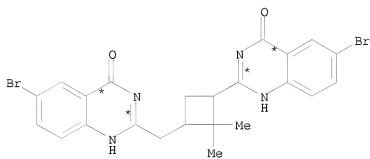


C



3 N

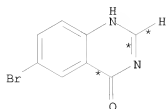
(7)



O

YIELD 50%

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P
YIELD 22%

RX(7) RCT C 517915-11-6, N 75-12-7

STAGE(1)

SOL 75-12-7 Formamide

CON SUBSTAGE(1) 2 hours, 180 - 185 deg C

SUBSTAGE(2) 185 deg C -> room temperature

STAGE(2)

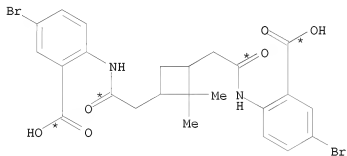
RGT Q 144-55-8 NaHCO₃

SOL 7732-18-5 Water

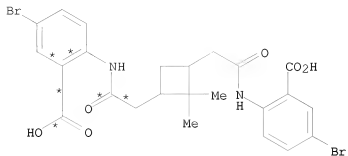
CON room temperature

PRO O 517915-17-2, P 32084-59-6

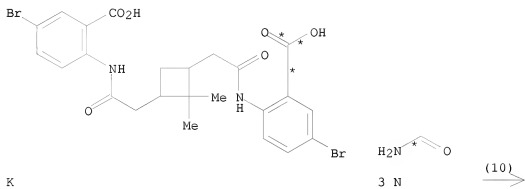
RX(10) OF 18 ...3 K + 3 N ==> W + P



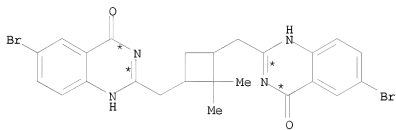
K



K

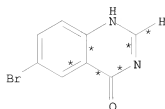


K



W

YIELD 48%



P
YIELD 19%

RX(10) RCT K 517915-14-9, N 75-12-7

STAGE(1)

SOL 75-12-7 Formamide
CON SUBSTAGE(1) 2 hours, 186 deg C
SUBSTAGE(2) 186 deg C -> room temperature

STAGE(2)

RGT Q 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON room temperature

PRO W 517915-20-7, P 32084-59-6

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 90 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 138:271640 CASREACT

TITLE: Synthesis of some new quinazoline-4-(3H)-ones and styryl hemicyanines as possible antimicrobial agents
AUTHOR(S): Afsah, S. A.; Ahmad, Jawaid; Purbey, R.; Kumar, A.
CORPORATE SOURCE: Post-graduate Department of Chemistry, R.K. College, Madhubani, 847 211, India

SOURCE: Asian Journal of Chemistry (2003), 15(1), 552-554
CODEN: AJCHEW; ISSN: 0970-7077

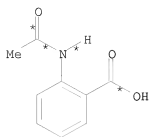
PUBLISHER: Asian Journal of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In the present note we report the synthesis of some new quinazoline-4 (3H)-ones and styryl hemicyanines as possible antimicrobial agents. The preparation and properties of the title styryl hemicyanines were not reported.

RX(2) OF 15 ...C + D ==> E

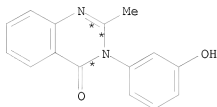


C



D

(2) \longrightarrow



E

YIELD 68%

RX(2) RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O

CON 4 - 6 hours, reflux

STAGE(2)

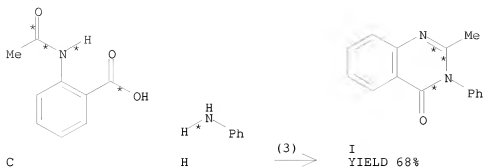
RCT D 591-27-5

SOL 64-19-7 AcOH

CON 4 - 6 hours, reflux

PRO E 40671-68-9

RX(3) OF 15 ...C + H ==> I



RX(3) RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O

CON 4 - 6 hours, reflux

STAGE(2)

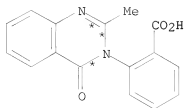
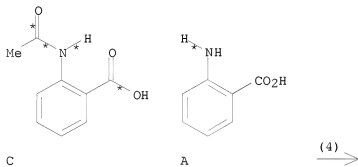
RCT H 62-53-3

SOL 64-19-7 AcOH

CON 4 - 6 hours, reflux

PRO I 2385-23-1

RX(4) OF 15 ...C + A ==> J



J
YIELD 68%

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RX(4) RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O

CON 4 - 6 hours, reflux

STAGE(2)

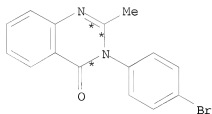
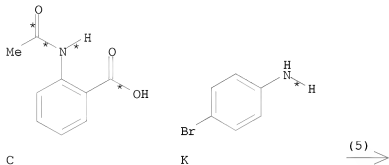
RCT A 118-92-3

SOL 64-19-7 AcOH

CON 4 - 6 hours, reflux

PRO J 4005-06-5

RX(5) OF 15 ...C + K ==> L



L
YIELD 68%

RX(5) RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O

CON 4 - 6 hours, reflux

STAGE(2)

RCT K 106-40-1

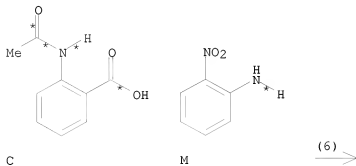
SOL 64-19-7 AcOH

CON 4 - 6 hours, reflux

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PRO L 1788-95-0

RX(6) OF 15 ...C + M ==> N



N
YIELD 68%

RX(6) RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O

CON 4 - 6 hours, reflux

STAGE(2)

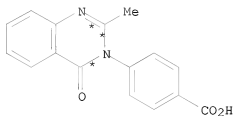
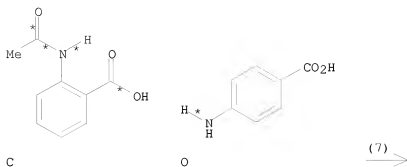
RCT M 88-74-4

SOL 64-19-7 AcOH

CON 4 - 6 hours, reflux

PRO N 1788-94-9

RX(7) OF 15 ...C + O ==> P



YIELD 68%

RX(7) RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O

CON 4 - 6 hours, reflux

STAGE(2)

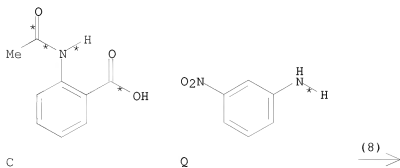
RCT O 150-13-0

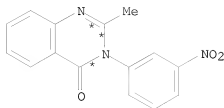
SOL 64-19-7 AcOH

CON 4 - 6 hours, reflux

PRO P 4005-05-4

RX(8) OF 15 ...C + Q ==> R





R
YIELD 68%

RX(8) RCT C 89-52-1

STAGE(1)

SOL 108-24-7 Ac2O
CON 4 - 6 hours, reflux

STAGE(2)

RCT Q 99-09-2
SOL 64-19-7 AcOH
CON 4 - 6 hours, reflux

PRO R 4309-26-6

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 91 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 138:239381 CASREACT

TITLE: Synthesis and application of some bisazo disperse dyes based on 4-hydroxyquinolinoquinazoline system on polyester fabric

AUTHOR(S): Patel, N. C.; Mehta, A. G.

CORPORATE SOURCE: Department of Chemistry, P.T. Sarvajani College of Science, Surat, 395 001, India

SOURCE: Journal of Indian Council of Chemists (2001), 18(2), 83-86

CODEN: JICCE7; ISSN: 0971-5037

PUBLISHER: Indian Council of Chemists

DOCUMENT TYPE: Journal

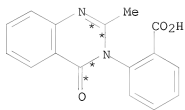
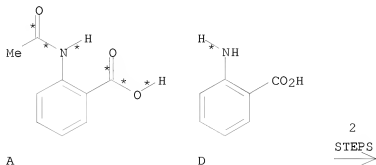
LANGUAGE: English

AB Ten 3-(4'-R-azo-1'-phenylazo)-4-hydroxyquinolino-[1,2-b]-4-oxoquinazolines were prepared by coupling diazotized 3-(4'-amino-1'-phenylazo)-4-hydroxyquinolino-[1,2-b]-4-oxoquinazoline with various coupling components. 4-Hydroxyquinolino-[1,2-b]-4-oxoquinazoline (I) was prepared by the condensation of 2-methyl-1,3-benzoxazin-8-one with anthranilic acid, giving initially 2-methyl-3-(1-carboxyphenyl)-4-oxoquinazoline followed by the ring closure. I was coupled with diazotized p-aminoacetanilide followed by hydrolysis to give 3-[4'-amino-1'-phenylazo]-4-hydroxyquinolino[1,2-b]-4-oxoquinazoline. The bisazo disperse dyes were characterized by elemental and spectral analyses and their dyeing performance on polyester fabric was

assessed. These compds. when applied on polyester fabric, gave shades with poor to good light fastness, very good to excellent wash fastness and poor to excellent exhaustion.

RX(16) OF 75 COMPOSED OF RX(1), RX(2)

RX(16) A + D ==> E



E
YIELD 85%

RX(1) RCT A 89-52-1
RGT C 108-24-7 Ac2O
PRO B 525-76-8
CON 30 minutes, reflux

RX(2) RCT B 525-76-8, D 118-92-3
PRO E 4005-06-5
SOL 64-19-7 AcOH
CON 3 hours, reflux

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 92 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 138:206465 CASREACT

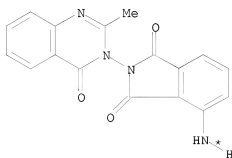
TITLE: Disperse dyes based on
2-methyl-3-[3'-aminophthalimido]-4(3H)-quinazolinone

AUTHOR(S): Patel, Vijay H.; Patel, Manish P.; Patel, Ranjan G.

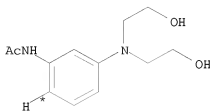
CORPORATE SOURCE: Department of Chemistry, Sardar Patel University,
Vallabh Vidyanagar, 388 120, India
SOURCE: Journal of the Serbian Chemical Society (2002),
67(11), 719-726
CODEN: JSCSEN; ISSN: 0352-5139
PUBLISHER: Serbian Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Azo heterocyclic disperse dyes were prepared by diazotization of 3-(3-aminophthalimido)-2-methyl-4(3H)-quinazolinone and coupling with 14 different mono- and di-N-substituted aniline derivs. The yellow to brown dyes were characterized by their percentage yield, m.p., UV-visible spectra, elemental anal., IR spectra, and dyeing performance on nylon 66 and polyester fibers. The percentage dye bath exhaustion was reasonably good and acceptable. The dyed fibers showed fair to fairly good to good fastness to light and very good to excellent fastness to washing, rubbing, perspiration, and sublimation.

RX(7) OF 29 ...A + Q ==> R



A



Q

(7) \longrightarrow

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(7) RCT A 500226-05-1

STAGE(1)

RGT D 7632-00-0 NaNO₂, E 7647-01-0 HCl
SOL 7732-18-5 Water
CON 0 - 5 deg C

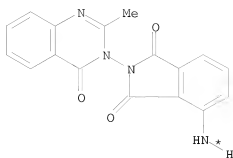
STAGE(2)

RCT Q 92-02-4
RGT E 7647-01-0 HCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) 45 minutes, 0 - 5 deg C
SUBSTAGE(2) 24 hours, 0 - 5 deg C, pH 5 - 6

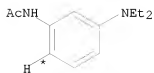
PRO R 500225-96-7

RX(13) OF 29 ...A + AC ==> AD

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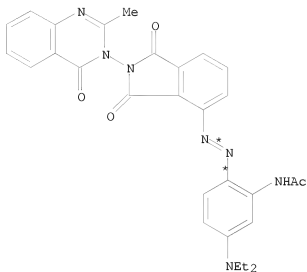


A



AC

(13)



AD

YIELD 75%

RX(13) RCT A 500226-05-1

STAGE(1)

RGT D 7632-00-0 NaNO2, E 7647-01-0 HCl

SOL 7732-18-5 Water

CON 0 - 5 deg C

STAGE(2)

RCT AC 6375-46-8

RGT E 7647-01-0 HCl

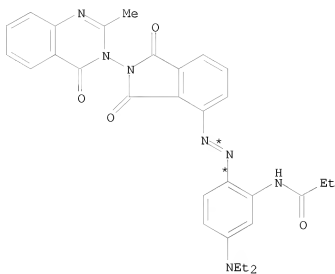
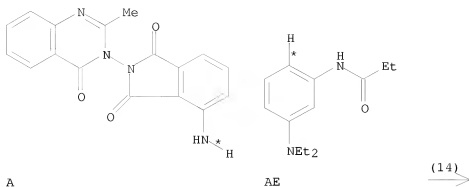
SOL 7732-18-5 Water

CON SUBSTAGE(1) 45 minutes, 0 - 5 deg C

SUBSTAGE(2) 24 hours, 0 - 5 deg C, pH 5 - 6

PRO AD 500226-02-8

RX(14) OF 29 ...A + AE ==> AF



YIELD 70%

RX(14) RCT A 500226-05-1

STAGE(1)

RGT D 7632-00-0 NaNO₂, E 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON 0 - 5 deg C

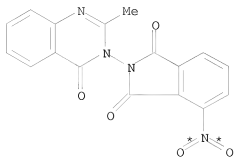
STAGE(2)

RCT AE 22185-75-7
 RGT E 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) 45 minutes, 0 - 5 deg C
 SUBSTAGE(2) 24 hours, 0 - 5 deg C, pH 5 - 6

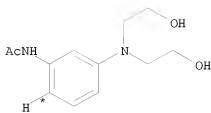
PRO AF 500226-03-9

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RX(22) OF 29 COMPOSED OF RX(15), RX(7)
RX(22) AG + Q ==> R



AG



Q

2
STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(15) RCT AG 500226-04-0

STAGE(1)

RGT E 7647-01-0 HCl, AH 7439-89-6 Fe
SOL 67-56-1 MeOH, 7732-18-5 Water
CON SUBSTAGE(1) 1 hour, reflux
SUBSTAGE(2) 2 hours, reflux

STAGE(2)

RGT AI 7664-41-7 NH3
SOL 7732-18-5 Water

PRO A 500226-05-1

RX(7) RCT A 500226-05-1

STAGE(1)

RGT D 7632-00-0 NaNO2, E 7647-01-0 HCl
SOL 7732-18-5 Water
CON 0 - 5 deg C

STAGE(2)

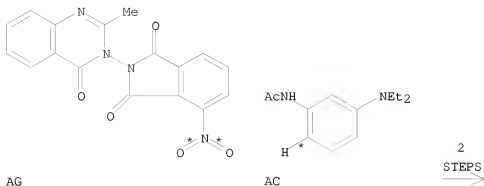
RCT Q 92-02-4
RGT E 7647-01-0 HCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) 45 minutes, 0 - 5 deg C
SUBSTAGE(2) 24 hours, 0 - 5 deg C, pH 5 - 6

PRO R 500225-96-7

RX(28) OF 29 COMPOSED OF RX(15), RX(13)

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RX(28) AG + AC ==> AD



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(15) RCT AG 500226-04-0

STAGE(1)

RGT E 7647-01-0 HCl, AH 7439-89-6 Fe

SOL 67-56-1 MeOH, 7732-18-5 Water

CON SUBSTAGE(1) 1 hour, reflux

SUBSTAGE(2) 2 hours, reflux

STAGE(2)

RGT AI 7664-41-7 NH3

SOL 7732-18-5 Water

PRO A 500226-05-1

RX(13) RCT A 500226-05-1

STAGE(1)

RGT D 7632-00-0 NaNO2, E 7647-01-0 HCl

SOL 7732-18-5 Water

CON 0 - 5 deg C

STAGE(2)

RCT AC 6375-46-8

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

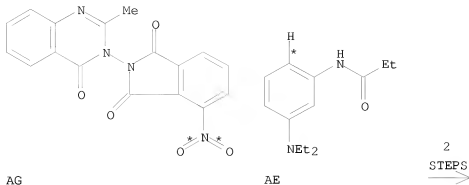
CON SUBSTAGE(1) 45 minutes, 0 - 5 deg C

SUBSTAGE(2) 24 hours, 0 - 5 deg C, pH 5 - 6

PRO AD 500226-02-8

RX(29) OF 29 COMPOSED OF RX(15), RX(14)

RX(29) AG + AE ==> AF



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(15) RCT AG 500226-04-0

STAGE(1)

RGT E 7647-01-0 HCl, AH 7439-89-6 Fe
SOL 67-56-1 MeOH, 7732-18-5 Water
CON SUBSTAGE(1) 1 hour, reflux
SUBSTAGE(2) 2 hours, reflux

STAGE(2)

RGT AI 7664-41-7 NH3
SOL 7732-18-5 Water

PRO A 500226-05-1

RX(14) RCT A 500226-05-1

STAGE(1)

RGT D 7632-00-0 NaNO2, E 7647-01-0 HCl
SOL 7732-18-5 Water
CON 0 - 5 deg C

STAGE(2)

RCT AE 22185-75-7
RGT E 7647-01-0 HCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) 45 minutes, 0 - 5 deg C
SUBSTAGE(2) 24 hours, 0 - 5 deg C, pH 5 - 6

PRO AF 500226-03-9

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 93 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

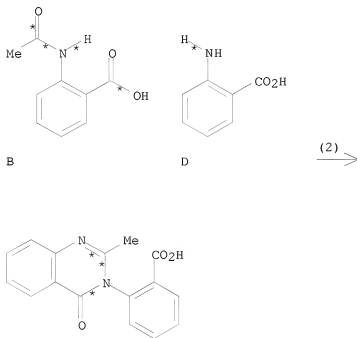
ACCESSION NUMBER: 138:122608 CASREACT

TITLE: Synthesis of derivatives of 4(3H)-quinazolinone with biological activities from N-acetylthranilic acid

AUTHOR(S): Nguyen, Ngoc Ninh; Truong, The Ky
 CORPORATE SOURCE: Institute of Testing, Ho Chi Minh City, Vietnam
 SOURCE: Tap Chi Duoc Hoc (2002), (1), 19-22
 CODEN: TCDHDQ; ISSN: 0258-6967
 PUBLISHER: Bo Y Te Xuat Ban
 DOCUMENT TYPE: Journal
 LANGUAGE: Vietnamese

AB 4(3H)-Quinazolinone derivs. were synthesized by the condensation of N-acetylanthranilic acid with aromatic amines or heteroarom. amines, resp. The obtained compds. were characterized by their m.p., elemental anal. data, and their mass, UV, IR, ¹H and ¹³C NMR spectra. The obtained derivs. of 4(3H)-quinazolinone were also biol. screened for hypnotic, analgesic, antibacterial and cytotoxic activities. 3-(2-Hydroxy-3-pyridinyl)-2-methyl-4(3H)-quinazolinone at 25 mg/kg showed analgesic activity in mice. No compds. showed hypnotic, cytotoxic and antibacterial activity.

RX(2) OF 15 ...B + D ==> E



E
 YIELD 62%

RX(2) RCT B 89-52-1, D 118-92-3

STAGE(1)

CON SUBSTAGE(1) 20 minutes, 150 - 160 deg C
 SUBSTAGE(2) 90 minutes, 160 deg C
 SUBSTAGE(3) 160 deg C -> 120 deg C

STAGE(2)

RGT C 7732-18-5 Water

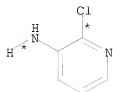
10/ 562,112

CON 120 deg C

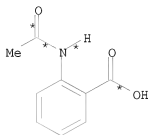
PRO E 4005-06-5

NTE polyphosphoric acid used as solvent

RX(4) OF 15 ...G + B ==> H

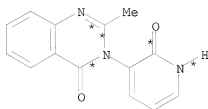


G



B

(4) \longrightarrow



H

YIELD 41%

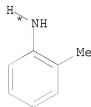
RX(4) RCT G 6298-19-7, B 89-52-1

PRO H 88369-51-1

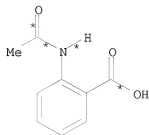
CON 180 deg C

NTE polyphosphoric acid used as solvent

RX(5) OF 15 ...I + B ==> J

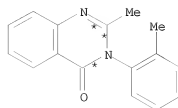


I



B

(5) \longrightarrow



J

YIELD 56%

10/ 562,112

RX(5) RCT I 95-53-4, B 89-52-1

STAGE(1)

CON SUBSTAGE(1) 20 minutes, 150 - 160 deg C
SUBSTAGE(2) 90 minutes, 160 deg C
SUBSTAGE(3) 160 deg C -> 120 deg C

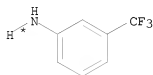
STAGE(2)

RGT C 7732-18-5 Water
CON 120 deg C

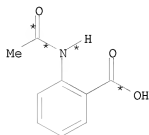
PRO J 72-44-6

NTE polyphosphoric acid used as solvent

RX(6) OF 15 ...K + B ==> L

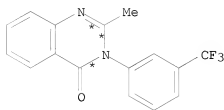


K



B

(6) \rightarrow



L

YIELD 73%

RX(6) RCT K 98-16-8, B 89-52-1

STAGE(1)

CON SUBSTAGE(1) 20 minutes, 150 - 160 deg C
SUBSTAGE(2) 90 minutes, 160 deg C
SUBSTAGE(3) 160 deg C -> 120 deg C

STAGE(2)

RGT C 7732-18-5 Water
CON 120 deg C

PRO L 1788-98-3

NTE polyphosphoric acid used as solvent

L3 ANSWER 94 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 138:14040 CASREACT

TITLE: Oxidation of 3-aminoquinazolinones with lead tetraacetate. A novel synthesis of naphtho-fused azirino-pyrazolo- and 1,4,5-oxadiazepinoquinazolinones

AUTHOR(S): El-Sharief, A. M. Sh.; Ammar, Y. A.; Zahran, M. A.; Ali, A. H.

CORPORATE SOURCE: Chemistry Department, Faculty of Science, Al-Azhar University, Cairo, Egypt

SOURCE: Journal of Chemical Research, Synopses (2002), (5), 205-208

CODEN: JRPSCD; ISSN: 0308-2342

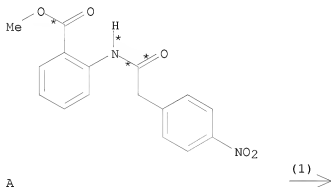
PUBLISHER: Science Reviews

DOCUMENT TYPE: Journal

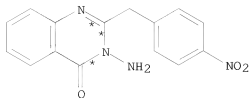
LANGUAGE: English

AB Oxidation of a 2-(arylmethyl)-3-Amino-4(3H)-quinazolinone derivs. using lead tetraacetate in methylene chloride at -20°C gave aziridine derivs. Oxidation of 2-(arylmethyl)-3-amino-4(3H)-quinazolinones gave aziridine derivs. Oxidation of 2-[(aryloxy)methyl]-3-amino-4(3H)-quinazolinones with lead tetraacetate under similar conditions gave the oxadiazepine derivs. 7H-naphtho[2',1':6,7][1,4,5]oxadiazepino[3,4-b]quinazolin-9(15H)-one and 16H-naphtho[1',2':6,7][1,4,5]oxadiazepino[3,4-b]quinazolin-14(8H)-one, resp.

RX(1) OF 26 A ==> B



A

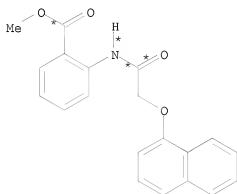


B

10/ 562,112

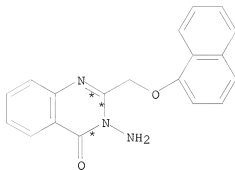
RX(1) RCT A 349410-48-6
RGT C 302-01-2 N2H4
PRO B 258524-94-6
SOL 71-36-3 BuOH
CON 4 - 6 hours, reflux

RX(8) OF 26 Q ==> R...



Q

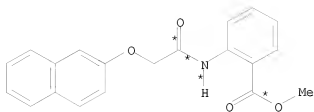
(8) \longrightarrow



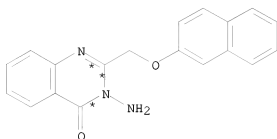
R

RX(8) RCT Q 420824-23-3
RGT C 302-01-2 N2H4
PRO R 477782-43-7
SOL 71-36-3 BuOH
CON 4 - 6 hours, reflux

RX(9) OF 26 S ==> T...



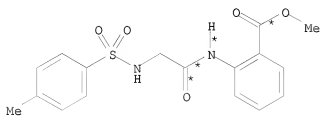
S

(9) \longrightarrow 

T

RX(9) RCT S 424800-39-5
 RGT C 302-01-2 N2H4
 PRO T 123798-73-2
 SOL 71-36-3 BuOH
 CON 4 - 6 hours, reflux

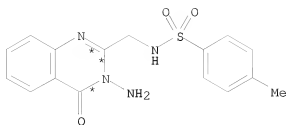
RX(12) OF 26 W ==> X...



W

(12) \longrightarrow

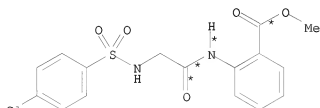
10/ 562,112



X

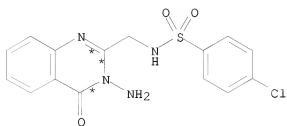
RX(12) RCT W 219970-85-1
 RGT C 302-01-2 N2H4
 PRO X 219970-93-1
 SOL 71-36-3 BuOH
 CON 4 - 6 hours, reflux

RX(13) OF 26 Y ==> Z...



Y

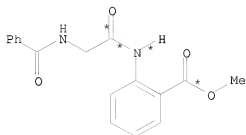
(13)



Z

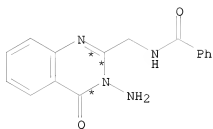
RX(13) RCT Y 219970-86-2
 RGT C 302-01-2 N2H4
 PRO Z 219970-94-2
 SOL 71-36-3 BuOH
 CON 4 - 6 hours, reflux

RX(14) OF 26 AA ==> AB...



AA

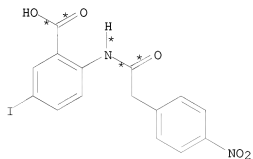
(14)
→



AB

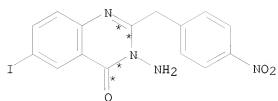
RX(14) RCT AA 219970-89-5
 RGT C 302-01-2 N2H4
 PRO AB 219970-96-4
 SOL 71-36-3 BuOH
 CON 4 - 6 hours, reflux

RX(18) OF 26 COMPOSED OF RX(2), RX(4)
 RX(18) E ==> J



E

2
STEPS
→

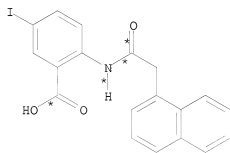


J

RX(2) RCT E 477782-35-7
 PRO F 477782-37-9
 SOL 108-24-7 Ac2O

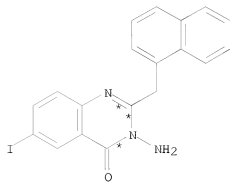
RX(4) RCT F 477782-37-9
 RGT C 302-01-2 N2H4
 PRO J 477782-39-1
 SOL 71-36-3 BuOH
 CON 4 - 6 hours, reflux

RX(19) OF 26 COMPOSED OF RX(3), RX(5)
 RX(19) H ==> K



H

2
 STEPS
 →



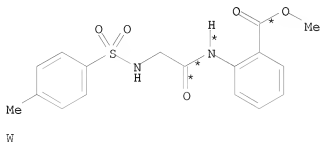
K

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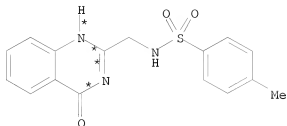
RX(3) RCT H 477782-36-8
PRO I 477782-38-0
SOL 108-24-7 Ac2O

RX(5) RCT I 477782-38-0
RGT C 302-01-2 N2H4
PRO K 477782-40-4
SOL 71-36-3 BuOH
CON 4 - 6 hours, reflux

RX(23) OF 26 COMPOSED OF RX(12), RX(15)
RX(23) W ==> AC



2
STEPS
→

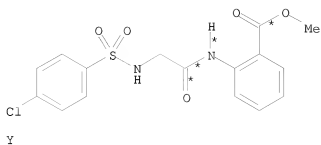


RX(12) RCT W 219970-85-1
RGT C 302-01-2 N2H4
PRO X 219970-93-1
SOL 71-36-3 BuOH
CON 4 - 6 hours, reflux

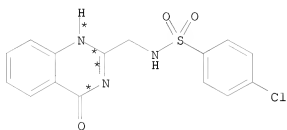
RX(15) RCT X 219970-93-1
RGT M 546-67-8 Pb(OAc)4
PRO AC 219971-11-6
SOL 75-09-2 CH2Cl2
CON -20 deg C

RX(24) OF 26 COMPOSED OF RX(13), RX(16)
RX(24) Y ==> AD

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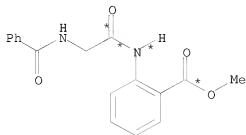
2
STEPS
→



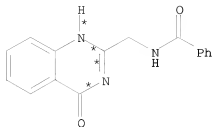
RX(13) RCT Y 219970-86-2
RGT C 302-01-2 N2H4
PRO Z 219970-94-2
SOL 71-36-3 BuOH
CON 4 - 6 hours, reflux

RX(16) RCT Z 219970-94-2
RGT M 546-67-8 Pb(OAc)4
PRO AD 219971-12-7
SOL 75-09-2 CH2Cl2
CON -20 deg C

RX(25) OF 26 COMPOSED OF RX(14), RX(17)
RX(25) AA ==> AE



2
STEPS
→



AE

RX(14) RCT AA 219970-89-5
 RGT C 302-01-2 NZH4
 PRO AB 219970-96-4
 SOL 71-36-3 BuOH
 CON 4 - 6 hours, reflux

RX(17) RCT AB 219970-96-4
 RGT M 546-67-8 Pb(OAc)₄
 PRO AE 219971-22-9
 SOL 75-09-2 CH₂Cl₂
 CON -20 deg C

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 95 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 137:279208 CASREACT

TITLE: Preparation of (indazol-5-ylamino)quinazolines as Rho-kinase inhibitors

INVENTOR(S): Nagarathnam, Dhanapalan; Asgari, Davoud; Shao, Jianxing; Liu, Xiao-Gao; Khire, Uday; Wang, Chunguang; Hart, Barry; Boyer, Stephen; Weber, Olaf; Lynch, Mark; Bankston, Donald

PATENT ASSIGNEE(S): Bayer Corporation, USA

SOURCE: PCI Int. Appl., 74 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002076976	A2	20021003	WO 2002-US8659	20020322
WO 2002076976	A3	20021212		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,			

	CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG	
CA 2441492	A1 20021003	CA 2002-2441492 20020322
AU 2002250394	A1 20021008	AU 2002-250394 20020322
US 20030125344	A1 20030703	US 2002-103566 20020322
EP 1370553	A2 20031217	EP 2002-719303 20020322
EP 1370553	B1 20060510	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR		
JP 2004524350	T 20040812	JP 2002-576234 20020322
AT 325795	T 20060615	AT 2002-719303 20020322
TW 261055	B 20060901	TW 2002-91105591 20020322
PT 1370553	T 20060929	PT 2002-719303 20020322
ES 2264477	T3 20070101	ES 2002-719303 20020322
US 20030220357	A1 20031127	US 2002-252369 20020924
CA 2507381	A1 20040408	CA 2003-2507381 20030924
WO 2004029045	A2 20040408	WO 2003-US29538 20030924
WO 2004029045	A3 20040722	
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW		
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG		
AU 2003270785	A1 20040419	AU 2003-270785 20030924
MX 2003008658	A 20050411	MX 2003-8658 20030924
EP 1542992	A2 20050622	EP 2003-752497 20030924
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK		
JP 2006508068	T 20060309	JP 2004-540124 20030924
EP 1953152	A1 20080806	EP 2008-103780 20030924
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LI, LU, MC, NL, PT, RO, SE, SI, SK, TR, AL, LT, LV, MK		
HK 1061030	A1 20060908	HK 2004-104115 20040609
MX 2005003273	A 20051018	MX 2005-3273 20050323
US 20060142313	A1 20060629	US 2006-354977 20060216
US 20060142314	A1 20060629	US 2006-354978 20060216
PRIORITY APPLN. INFO.:		US 2001-277974P 20010323
		US 2001-315341P 20010829
		US 2001-315338P 20010829
		US 2002-103565 20020322
		US 2002-103566 20020322
		WO 2002-US8659 20020322
		US 2002-252369 20020924
		EP 2003-752497 20030924
		WO 2003-US29538 20030924

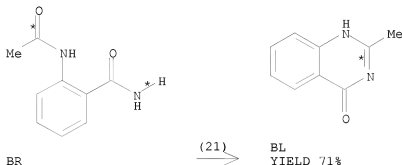
OTHER SOURCE(S): MARPAT 137:279208
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [Y = N, CR17; X = alkyl, alkoxy, thioalkoxy, amido, etc.; p = 0-3; a, c = CR5, NR6, etc.; b = CR5, N; A = H, halo, carboxy, cyano,

alkoxy, etc.; B = (un)substituted up to 3 times in any position by R5; R1,6 = H, alkyl; R2-5 = H, alkyl, alkenyl; R17 = H, alkyl, CN with provisions] were prepared. For instance, 2,4-Dichloroquinazoline (preparation given) was reacted with 5-aminoindazole (THF/H₂O, KOAc) to give 2-(N-(1H-indazol-5-yl)amino)-4-chloroquinazoline in 92% yield. This was coupled to 2,4-dichlorophenylboronic acid (ethylene glycol di-Me ether, Pd(dppf)Cl₂, NaHCO₃, reflux) to give II. I are rho-kinase inhibitors and are useful for inhibiting tumor growth, treating erectile dysfunction and coronary heart disease.

RX(21) OF 174 ...BR ==> BL...



RX(21) RCT BR 33809-77-7
RGT AF 1310-73-2 NaOH
PRO BL 1769-24-0
SOL 7732-18-5 Water, 64-17-5 EtOH

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 96 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 137:247841 CASREACT

TITLE: Oxygen analogs of the benzodiazepine alkaloids sclerotigenin and circumdatin F

AUTHOR(S): Witt, Anette; Bergman, Jan

CORPORATE SOURCE: Unit for Organic Chemistry, Department of Biosciences, Novum Research Park, Karolinska Institute and Södertörn University College, Huddinge, SE-141 57, Swed.

SOURCE: Journal of Heterocyclic Chemistry (2002), 39(2), 351-355

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

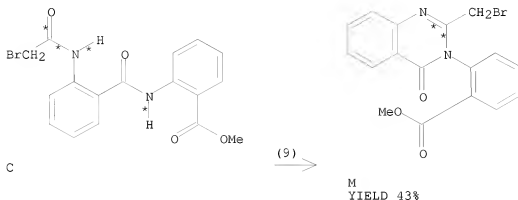
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new type of fused oxazepinones, which are analogs of sclerotigenin and circumdatin F, were obtained in a two step synthesis from 2-(2-amino-benzoylamino)benzoic acid or the corresponding Me ester. Secondly a new synthesis of circumdatin F arose from this work, where 2-(2-propionylaminobenzoylamino)benzoic acid Me ester was used as an intermediate.

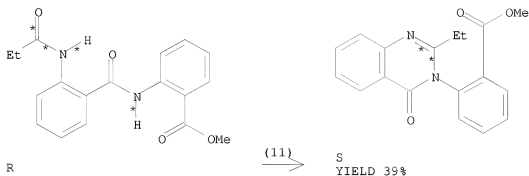
10/ 562,112

RX(9) OF 29 ...C ==> M...



RX(9) RCT C 460062-20-8
PRO M 61554-52-7
CAT 104-15-4 TsOH
SOL 108-88-3 PhMe
CON 60 hours, reflux

RX(11) OF 29 ...R ==> S...



RX(11) RCT R 460062-44-6

STAGE(1)
SOL 68-12-2 DMF
CON 65 hours, reflux

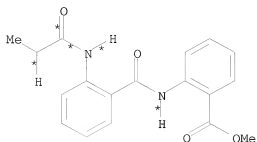
STAGE(2)
RGT U 7732-18-5 Water
CON 1 hour

PRO S 94209-49-1

RX(23) OF 29 COMPOSED OF RX(11), RX(12)

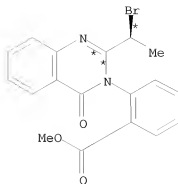
10/ 562,112

RX(23) 2 R ==> V + W

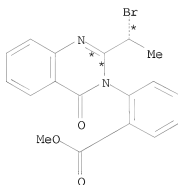


2 R

2
STEPS
→



V
YIELD 47%



W
YIELD 32%

RX(11) RCT R 460062-44-6

STAGE(1)

SOL 68-12-2 DMF

CON 65 hours, reflux

STAGE(2)

RGT U 7732-18-5 Water

CON 1 hour

PRO S 94209-49-1

RX(12)

RCT S 94209-49-1

RGT X 127-09-3 AcONa, Y 7726-95-6 Br₂

PRO V 460062-47-9, W 460062-48-0

SOL 7732-18-5 Water, 64-19-7 AcOH

CON SUBSTAGE(1) 15 minutes, 60 deg C

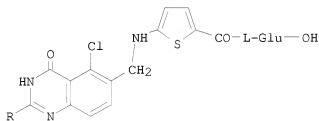
SUBSTAGE(2) 1.5 hours

NTE stereoselective, overall yield of distereomeric mixture = 87%

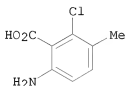
and ratio is 7:3

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 97 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 137:185777 CASREACT
 TITLE: Synthesis and In Vitro Antitumor Activity of Thiophene Analogues of 5-Chloro-5,8-dideazafoolic Acid and 2-Methyl-2-desamino-5-chloro-5,8-dideazafoolic Acid
 AUTHOR(S): Forsch, Ronald A.; Wright, Joel E.; Rosowsky, Andre
 CORPORATE SOURCE: Dana-Farber Cancer Institute and the Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA
 SOURCE: Bioorganic & Medicinal Chemistry (2002), 10(6), 2067-2076
 CODEN: BMECEP; ISSN: 0968-0896
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



I

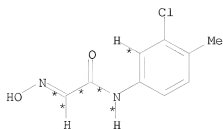


III

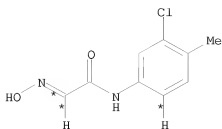
AB N-[5-[N-(2-Amino-5-chloro-3,4-dihydro-4-oxoquinazolin-6-yl)methylamino]-2-thenoyl]-L-glutamic acid (I; R = NH₂) and N-[5-[N-(5-chloro-3,4-dihydro-2-methyl-4-oxoquinazolin-6-yl)methylamino]-2-thenoyl]-L-glutamic acid (I; R = Me), the first reported thiophene analogs of 5-chloro-5,8-dideazafoolic acid, were synthesized and tested as inhibitors of tumor cell growth in culture. 4-Chloro-5-methylisatin was converted stepwise to Me 2-amino-5-methyl-6-chlorobenzoate and 2-amino-5-chloro-3,4-dihydro-6-methyl-4-oxoquinazoline. Pivaloylation of the 2-amino group, followed by NBS bromination, condensation with di-tert-Bu N-(5-amino-2-thenoyl)-L-glutamate (II), and stepwise cleavage of the protecting groups with ammonia and TFA yielded I (R = NH₂). Treatment of (III) with acetic anhydride afforded 2,6-dimethyl-5-chlorobenz[1,3-d]oxazin-4-one, which on reaction with ammonia, NaOH was converted to 2,6-dimethyl-5-chloro-3,4-dihydroquinazolin-4-one (IV). Bromination of IV, followed by condensation with 28 and ester cleavage with TFA, yielded I (R = Me). The IC₅₀ of I (R = NH₂ or Me) against CCRF-CEM human leukemic lymphoblasts was 1.8±0.1 and 2.1±0.8 μM, resp.

RX(53) OF 209 COMPOSED OF RX(3), RX(6), RX(8), RX(18)
 RX(53) 2 I + W ==> BC

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I

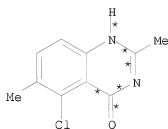


I



W

4
STEPS
→



BC
YIELD 99%

RX(3) RCT I 155184-79-5

STAGE(1)

RGT N 7664-93-9 H2SO4

STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)

RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2

SOL 7732-18-5 Water

STAGE(2)

RGT S 7647-01-0 HCl

SOL 7732-18-5 Water

PRO P 155184-82-0

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RX(8) RCT P 155184-82-0, W 108-24-7
 PRO X 450407-91-7
 SOL 108-24-7 Ac2O

RX(18) RCT X 450407-91-7

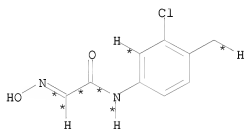
STAGE(1)
 RGT BB 7664-41-7 NH3

STAGE(2)
 RGT Q 1310-73-2 NaOH
 SOL 7732-18-5 Water

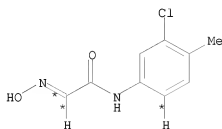
STAGE(3)
 RGT O 64-19-7 AcOH

PRO BC 450407-92-8

RX(93) OF 209 COMPOSED OF RX(3), RX(6), RX(8), RX(18), RX(19)
 RX(93) 2 I + W ==> BD



I

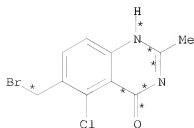


I



W

5
 STEPS
 →



BD
 YIELD 77%

RX(3) RCT I 155184-79-5
STAGE(1)
RGT N 7664-93-9 H2SO4
STAGE(2)
SOL 67-64-1 Me2CO
PRO L 53003-18-2, M 96187-75-6

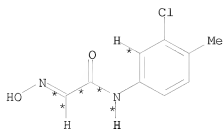
RX(6) RCT L 53003-18-2
STAGE(1)
RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2
SOL 7732-18-5 Water
STAGE(2)
RGT S 7647-01-0 HCl
SOL 7732-18-5 Water
PRO P 155184-82-0

RX(8) RCT P 155184-82-0, W 108-24-7
PRO X 450407-91-7
SOL 108-24-7 Ac2O

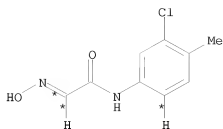
RX(18) RCT X 450407-91-7
STAGE(1)
RGT BB 7664-41-7 NH3
STAGE(2)
RGT Q 1310-73-2 NaOH
SOL 7732-18-5 Water
STAGE(3)
RGT O 64-19-7 AcOH
PRO BC 450407-92-8

RX(19) RCT BC 450407-92-8
RGT AN 128-08-5 Bromosuccinimide
PRO BD 450407-93-9
CAT 94-36-0 Benzoyl peroxide
SOL 67-66-3 CHCl3

RX(99) OF 209 COMPOSED OF RX(3), RX(6), RX(8), RX(18), RX(19), RX(20)
RX(99) 2 I + W + AU ==> BE



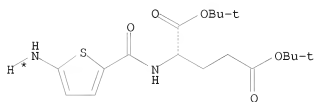
I



I

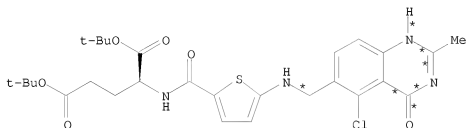


W



AU

6
STEPS
→



BE

RX(3) RCT I 155184-79-5

STAGE(1)

RGT N 7664-93-9 H2SO4

STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)

RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2

SOL 7732-18-5 Water

STAGE(2)

RGT S 7647-01-0 HCl

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SOL 7732-18-5 Water

PRO P 155184-82-0

RX(8) RCT P 155184-82-0, W 108-24-7
PRO X 450407-91-7
SOL 108-24-7 Ac2O

RX(18) RCT X 450407-91-7

STAGE(1)

RGT BB 7664-41-7 NH3

STAGE(2)

RGT Q 1310-73-2 NaOH

SOL 7732-18-5 Water

STAGE(3)

RGT O 64-19-7 AcOH

PRO BC 450407-92-8

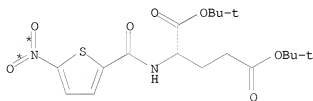
RX(19) RCT BC 450407-92-8
RGT AN 128-08-5 Bromosuccinimide
PRO BD 450407-93-9
CAT 94-36-0 Benzoyl peroxide
SOL 67-66-3 CHCl3

RX(20) RCT BD 450407-93-9, AU 132463-36-6
RGT AZ 144-55-8 NaHCO3
PRO BE 450407-94-0
SOL 68-12-2 DMF

RX(110) OF 209 COMPOSED OF REACTION SEQUENCE RX(15), RX(20)
AND REACTION SEQUENCE RX(3), RX(6), RX(8), RX(18), RX(19),
RX(20)

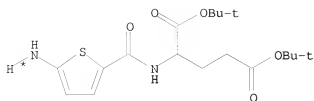
...AR ==> AU...

...2 I + W + AU ==> BE



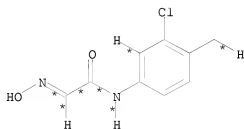
AR

6
STEPS
→

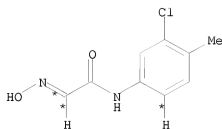


AU

START NEXT REACTION SEQUENCE



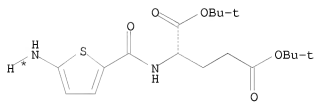
I



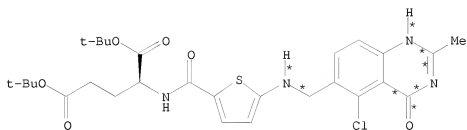
I



W



AU

6
STEPS
→

BE

RX(15) RCT AR 450407-87-1
 RGT AV 7439-89-6 Fe
 PRO AU 132463-36-6
 CAT 7720-78-7 FeSO4
 SOL 67-56-1 MeOH

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RX(3) RCT I 155184-79-5

STAGE(1)

RGT N 7664-93-9 H2SO4

STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)

RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2

SOL 7732-18-5 Water

STAGE(2)

RGT S 7647-01-0 HCl

SOL 7732-18-5 Water

PRO P 155184-82-0

RX(8) RCT P 155184-82-0, W 108-24-7

PRO X 450407-91-7

SOL 108-24-7 Ac2O

RX(18) RCT X 450407-91-7

STAGE(1)

RGT BB 7664-41-7 NH3

STAGE(2)

RGT Q 1310-73-2 NaOH

SOL 7732-18-5 Water

STAGE(3)

RGT O 64-19-7 AcOH

PRO BC 450407-92-8

RX(19) RCT BC 450407-92-8

RGT AN 128-08-5 Bromosuccinimide

PRO BD 450407-93-9

CAT 94-36-0 Benzoyl peroxide

SOL 67-66-3 CHCl3

RX(20) RCT BD 450407-93-9, AU 132463-36-6

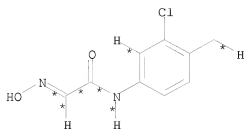
RGT AZ 144-55-8 NaHCO3

PRO BE 450407-94-0

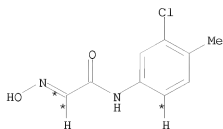
SOL 68-12-2 DMF

RX(111) OF 209 COMPOSED OF RX(3), RX(6), RX(8), RX(18), RX(19), RX(20), RX(21)

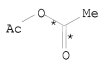
RX(111) 2 I + W + AU ==> BF



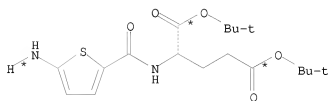
I



I

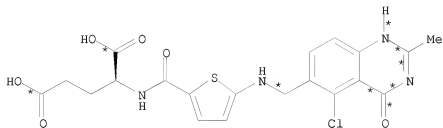


W



AU

7
STEPS
→



BF

YIELD 39%

RX(3) RCT I 155184-79-5

STAGE(1)

RGT N 7664-93-9 H2SO4

STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)

RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2

SOL 7732-18-5 Water

```

      STAGE(2)
      RGT  S 7647-01-0 HCl
      SOL  7732-18-5 Water

PRO  P 155184-82-0

RX(8)  RCT  P 155184-82-0, W 108-24-7
      PRO  X 450407-91-7
      SOL  108-24-7 Ac2O

RX(18) RCT  X 450407-91-7

      STAGE(1)
      RGT  BB 7664-41-7 NH3

      STAGE(2)
      RGT  Q 1310-73-2 NaOH
      SOL  7732-18-5 Water

      STAGE(3)
      RGT  O 64-19-7 AcOH

PRO  BC 450407-92-8

RX(19) RCT  BC 450407-92-8
      RGT  AN 128-08-5 Bromosuccinimide
      PRO  BD 450407-93-9
      CAT  94-36-0 Benzoyl peroxide
      SOL  67-66-3 CHCl3

RX(20) RCT  BD 450407-93-9, AU 132463-36-6
      RGT  AZ 144-55-8 NaHCO3
      PRO  BE 450407-94-0
      SOL  68-12-2 DMF

RX(21) RCT  BE 450407-94-0

      STAGE(1)
      RGT  AD 76-05-1 F3CCO2H
      SOL  75-09-2 CH2Cl2

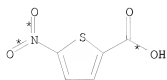
      STAGE(2)
      RGT  Q 1310-73-2 NaOH
      SOL  7732-18-5 Water

      STAGE(3)
      RGT  O 64-19-7 AcOH

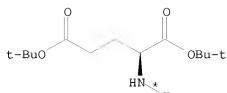
PRO  BF 450407-96-2

RX(158) OF 209 COMPOSED OF REACTION SEQUENCE RX(14), RX(15), RX(20)
      AND REACTION SEQUENCE RX(3), RX(6), RX(8), RX(18), RX(19),
      RX(20)
...B  +  AQ  ==>  AU...
...2 I  +  W  +  AU  ==>  BE

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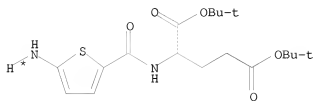


B



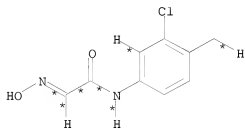
AQ

6
STEPS
→

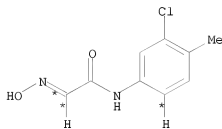


AU

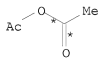
START NEXT REACTION SEQUENCE



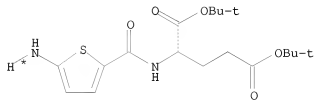
I



I

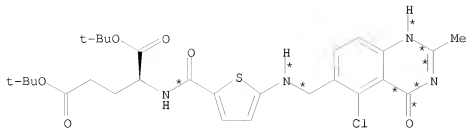


W



AU

6
STEPS
→



BE

RX(14) RCT B 6317-37-9

STAGE(1)

RGT AS 7719-09-7 SOC12

STAGE(2)

RCT AQ 16874-06-9

SOL 75-09-2 CH2Cl2

STAGE(3)

RGT AK 121-44-8 Et3N

PRO AR 450407-87-1

RX(15)

RCT AR 450407-87-1

RGT AV 7439-89-6 Fe

PRO AU 132463-36-6

CAT 7720-78-7 FeSO4

SOL 67-56-1 MeOH

RX(3)

RCT I 155184-79-5

STAGE(1)

RGT N 7664-93-9 H2SO4

STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6)

RCT L 53003-18-2

STAGE(1)

RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2

SOL 7732-18-5 Water

STAGE(2)

RGT S 7647-01-0 HCl

SOL 7732-18-5 Water

PRO P 155184-82-0

RX(8)

RCT P 155184-82-0, W 108-24-7

PRO X 450407-91-7

SOL 108-24-7 Ac2O

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RX(18) RCT X 450407-91-7

STAGE(1)

RGT BB 7664-41-7 NH3

STAGE(2)

RGT Q 1310-73-2 NaOH

SOL 7732-18-5 Water

STAGE(3)

RGT O 64-19-7 AcOH

PRO BC 450407-92-8

RX(19) RCT BC 450407-92-8
RGT AN 128-08-5 Bromosuccinimide
PRO BD 450407-93-9
CAT 94-36-0 Benzoyl peroxide
SOL 67-66-3 CHCl3

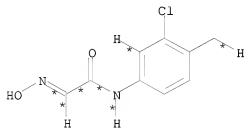
RX(20) RCT BD 450407-93-9, AU 132463-36-6
RGT AZ 144-55-8 NaHCO3
PRO BE 450407-94-0
SOL 68-12-2 DMF

RX(167) OF 209 COMPOSED OF REACTION SEQUENCE RX(3), RX(6), RX(8), RX(18),
RX(19), RX(20)

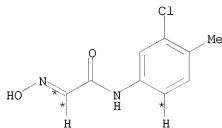
AND REACTION SEQUENCE RX(1), RX(14), RX(15), RX(20)

...2 I + W ==> BD...

...A + AQ + BD ==> BE



I

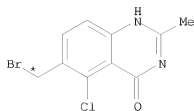


I



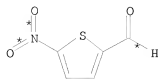
W

4
STEPS
→

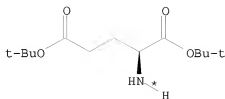


BD

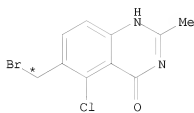
START NEXT REACTION SEQUENCE



A

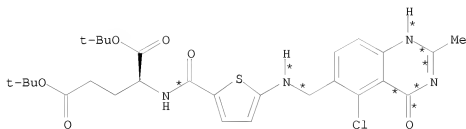


AQ



BD

4
STEPS
→



BE

RX(3) RCT I 155184-79-5

STAGE(1)

RGT N 7664-93-9 H2SO4

STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)

RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2

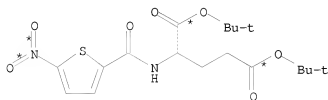
SOL 7732-18-5 Water

STAGE(2)
RGT S 7647-01-0 HCl
SOL 7732-18-5 Water
PRO P 155184-82-0
RX(8) RCT P 155184-82-0, W 108-24-7
PRO X 450407-91-7
SOL 108-24-7 Ac2O
RX(18) RCT X 450407-91-7
STAGE(1)
RGT BB 7664-41-7 NH3
STAGE(2)
RGT Q 1310-73-2 NaOH
SOL 7732-18-5 Water
STAGE(3)
RGT O 64-19-7 AcOH
PRO BC 450407-92-8
RX(19) RCT BC 450407-92-8
RGT AN 128-08-5 Bromosuccinimide
PRO BD 450407-93-9
CAT 94-36-0 Benzoyl peroxide
SOL 67-66-3 CHCl3
RX(1) RCT A 4521-33-9
RGT C 7722-64-7 KMnO4, D 7558-80-7 NaH2PO4
PRO B 6317-37-9
SOL 7732-18-5 Water, 67-64-1 Me2CO
RX(14) RCT B 6317-37-9
STAGE(1)
RGT AS 7719-09-7 SOCl2
STAGE(2)
RCT AQ 16874-06-9
SOL 75-09-2 CH2Cl2
STAGE(3)
RGT AK 121-44-8 Et3N
PRO AR 450407-87-1
RX(15) RCT AR 450407-87-1
RGT AV 7439-89-6 Fe
PRO AU 132463-36-6
CAT 7720-78-7 FeSO4
SOL 67-56-1 MeOH
RX(20) RCT BD 450407-93-9, AU 132463-36-6
RGT AZ 144-55-8 NaHCO3
PRO BE 450407-94-0
SOL 68-12-2 DMF

RX(173) OF 209 COMPOSED OF REACTION SEQUENCE RX(15), RX(20), RX(21)
AND REACTION SEQUENCE RX(3), RX(6), RX(8), RX(18), RX(19),
RX(20), RX(21)

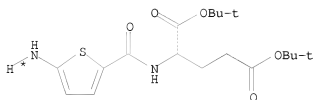
...AR ==> AU...

...2 I + W + AU ==> BF



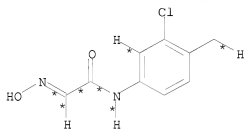
AR

7
STEPS
→

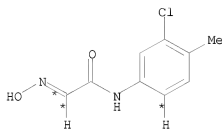


AU

START NEXT REACTION SEQUENCE



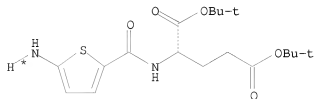
I



I



W



AU

7
STEPS
→

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PRO BC 450407-92-8

RX(19) RCT BC 450407-92-8
RGT AN 128-08-5 Bromosuccinimide
PRO BD 450407-93-9
CAT 94-36-0 Benzoyl peroxide
SOL 67-66-3 CHCl3

RX(20) RCT BD 450407-93-9, AU 132463-36-6
RGT AZ 144-55-8 NaHCO3
PRO BE 450407-94-0
SOL 68-12-2 DMF

RX(21) RCT BE 450407-94-0

STAGE(1)

RGT AD 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT Q 1310-73-2 NaOH
SOL 7732-18-5 Water

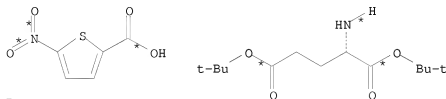
STAGE(3)

RGT O 64-19-7 AcOH

PRO BF 450407-96-2

RX(174) OF 209 COMPOSED OF REACTION SEQUENCE RX(14), RX(15), RX(20), RX(21)
AND REACTION SEQUENCE RX(3), RX(6), RX(8), RX(18), RX(19),
RX(20), RX(21)

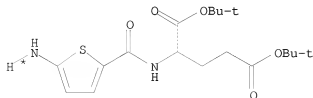
...B + AQ ==> AU...
...2 I + W + AU ==> BF



B

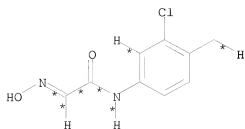
AQ

7
STEPS
➔

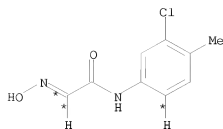


AU

START NEXT REACTION SEQUENCE



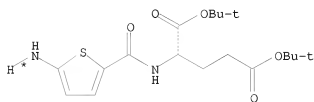
I



I

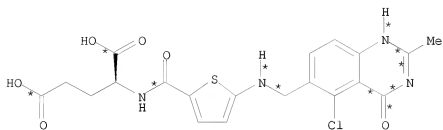


W



AU

7
STEPS
→



BF

YIELD 39%

RX(14) RCT B 6317-37-9

STAGE(1)

RGT AS 7719-09-7 SOCl2

STAGE(2)

RCT AQ 16874-06-9

SOL 75-09-2 CH2Cl2

STAGE(3)

RGT AK 121-44-8 Et3N

PRO AR 450407-87-1

RX(15) RCT AR 450407-87-1
RGT AV 7439-89-6 Fe
PRO AU 132463-36-6

CAT 7720-78-7 FeSO4
SOL 67-56-1 MeOH

RX(3) RCT I 155184-79-5
STAGE(1)
RGT N 7664-93-9 H2SO4
STAGE(2)
SOL 67-64-1 Me2CO
PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2
STAGE(1)
RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2
SOL 7732-18-5 Water
STAGE(2)
RGT S 7647-01-0 HCl
SOL 7732-18-5 Water
PRO P 155184-82-0

RX(8) RCT P 155184-82-0, W 108-24-7
PRO X 450407-91-7
SOL 108-24-7 Ac2O

RX(18) RCT X 450407-91-7
STAGE(1)
RGT BB 7664-41-7 NH3
STAGE(2)
RGT Q 1310-73-2 NaOH
SOL 7732-18-5 Water
STAGE(3)
RGT O 64-19-7 AcOH
PRO BC 450407-92-8

RX(19) RCT BC 450407-92-8
RGT AN 128-08-5 Bromosuccinimide
PRO BD 450407-93-9
CAT 94-36-0 Benzoyl peroxide
SOL 67-66-3 CHCl3

RX(20) RCT BD 450407-93-9, AU 132463-36-6
RGT AZ 144-55-8 NaHCO3
PRO BE 450407-94-0
SOL 68-12-2 DMF

RX(21) RCT BE 450407-94-0
STAGE(1)
RGT AD 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2

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STAGE(2)

RGT Q 1310-73-2 NaOH

SOL 7732-18-5 Water

STAGE(3)

RGT O 64-19-7 AcOH

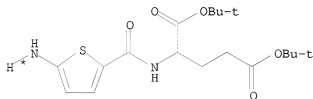
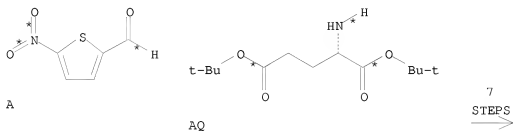
PRO BF 450407-96-2

RX(189) OF 209 COMPOSED OF REACTION SEQUENCE RX(1), RX(14), RX(15), RX(20),
RX(21)

AND REACTION SEQUENCE RX(3), RX(6), RX(8), RX(18), RX(19),
RX(20), RX(21)

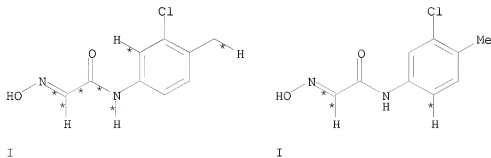
...A + AQ ==> AU...

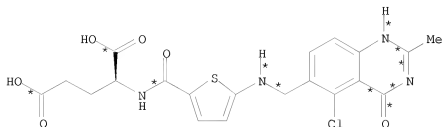
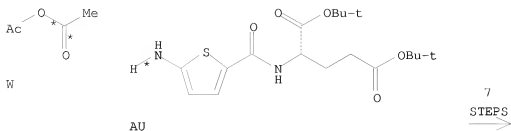
...2 I + W + AU ==> BF



AU

START NEXT REACTION SEQUENCE





BF
YIELD 39%

RX(1) RCT A 4521-33-9
RGT C 7722-64-7 KMnO₄, D 7558-80-7 NaH₂PO₄
PRO B 6317-37-9
SOL 7732-18-5 Water, 67-64-1 Me₂CO

RX(14) RCT B 6317-37-9
STAGE(1)
RGT AS 7719-09-7 SOCl₂

STAGE(2)
RCT AQ 16874-06-9
SOL 75-09-2 CH₂Cl₂

STAGE(3)
RGT AK 121-44-8 Et₃N

PRO AR 450407-87-1

RX(15) RCT AR 450407-87-1
RGT AV 7439-89-6 Fe
PRO AU 132463-36-6
CAT 7720-78-7 FeSO₄
SOL 67-56-1 MeOH

RX(3) RCT I 155184-79-5
STAGE(1)
RGT N 7664-93-9 H₂SO₄
STAGE(2)

SOL 67-64-1 Me2CO

PRO L 53003-18-2, M 96187-75-6

RX(6) RCT L 53003-18-2

STAGE(1)
RGT Q 1310-73-2 NaOH, R 7722-84-1 H2O2
SOL 7732-18-5 Water

STAGE(2)
RGT S 7647-01-0 HCl
SOL 7732-18-5 Water

PRO P 155184-82-0

RX(8) RCT P 155184-82-0, W 108-24-7
PRO X 450407-91-7
SOL 108-24-7 Ac2O

RX(18) RCT X 450407-91-7

STAGE(1)
RGT BB 7664-41-7 NH3

STAGE(2)
RGT Q 1310-73-2 NaOH
SOL 7732-18-5 Water

STAGE(3)
RGT O 64-19-7 AcOH

PRO BC 450407-92-8

RX(19) RCT BC 450407-92-8
RGT AN 128-08-5 Bromosuccinimide
PRO BD 450407-93-9
CAT 94-36-0 Benzoyl peroxide
SOL 67-66-3 CHCl3

RX(20) RCT BD 450407-93-9, AU 132463-36-6
RGT AZ 144-55-8 NaHCO3
PRO BE 450407-94-0
SOL 68-12-2 DMF

RX(21) RCT BE 450407-94-0

STAGE(1)
RGT AD 76-05-1 F3CCO2H
SOL 75-09-2 CH2Cl2

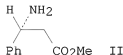
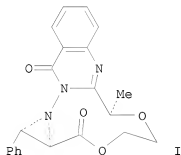
STAGE(2)
RGT Q 1310-73-2 NaOH
SOL 7732-18-5 Water

STAGE(3)
RGT O 64-19-7 AcOH

PRO BF 450407-96-2

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

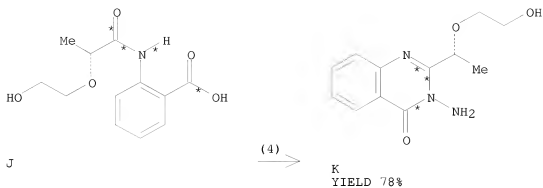
L3 ANSWER 98 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 137:154915 CASREACT
 TITLE: Completely diastereoselective aziridination of α,β -unsaturated acids via intramolecular reaction of 3-acetoxyaminoquinazolin-4(3H)-ones
 AUTHOR(S): Atkinson, Robert S.; Draycott, Richard D.; Hirst, David J.; Parratt, Martin J.; Raynham, Tony M.
 CORPORATE SOURCE: Department of Chemistry, Leicester University, Leicester, LE1 7RH, UK
 SOURCE: Tetrahedron Letters (2002), 43(11), 2083-2085
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB (R)-3-Amino-2-[1-(2-hydroxyethoxy)ethyl]quinazolin-4(3H)-one was prepared in 62% yield without the need for chromatog. and O-cinnamoylated; reaction with lead tetraacetate gave aziridine I as a single diastereoisomer in quant. yield which was converted into the β -amino acid ester II corresponding to overall enantioselective addition of ammonia to the double bond of cinnamic acid.

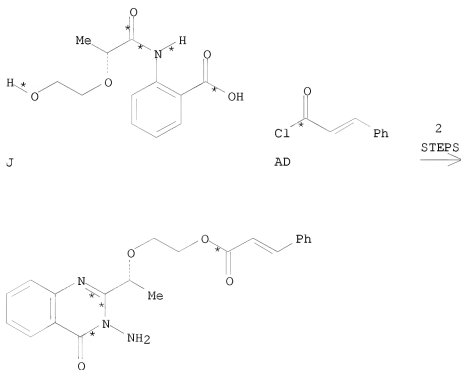
RX(4) OF 54 ...J ==> K...

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RX(4) RCT J 445397-15-9
 RGT L 302-01-2 N2H4
 PRO K 445397-14-8
 SOL 64-17-5 EtOH

RX(16) OF 54 COMPOSED OF RX(4), RX(8)
 RX(16) J + AD ==> AE



AE
 YIELD 91%

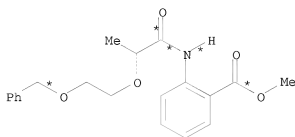
RX(4) RCT J 445397-15-9
 RGT L 302-01-2 N2H4

10/ 562,112

PRO K 445397-14-8
SOL 64-17-5 EtOH

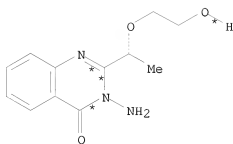
RX(8) RCT K 445397-14-8, AD 17082-09-6
RGT Z 110-86-1 Pyridine
PRO AE 445397-17-1
SOL 75-09-2 CH2Cl2

RX(18) OF 54 COMPOSED OF RX(6), RX(4)
RX(18) S ==> K



S

2
STEPS
→

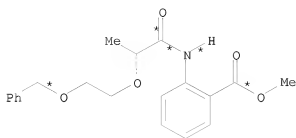


K
YIELD 78%

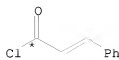
RX(6) RCT S 445397-16-0
RGT T 1333-74-0 H2
PRO J 445397-15-9
CAT 7440-05-3 Pd
SOL 64-19-7 AcOH

RX(4) RCT J 445397-15-9
RGT L 302-01-2 N2H4
PRO K 445397-14-8
SOL 64-17-5 EtOH

RX(30) OF 54 COMPOSED OF RX(6), RX(4), RX(8)
RX(30) S + AD ==> AE

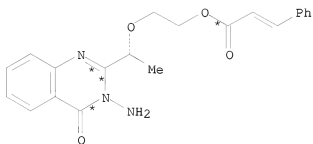


S



AD

3
STEPS
→



AE

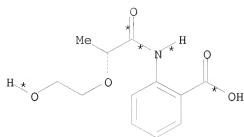
YIELD 91%

RX(6) RCT S 445397-16-0
RGT T 1333-74-0 H2
PRO J 445397-15-9
CAT 7440-05-3 Pd
SOL 64-19-7 AcOH

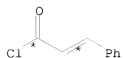
RX(4) RCT J 445397-15-9
RGT L 302-01-2 N2H4
PRO K 445397-14-8
SOL 64-17-5 EtOH

RX(8) RCT K 445397-14-8, AD 17082-09-6
RGT Z 110-86-1 Pyridine
PRO AE 445397-17-1
SOL 75-09-2 CH2Cl2

RX(40) OF 54 COMPOSED OF RX(4), RX(8), RX(9), RX(10), RX(11)
RX(40) J + AD + AA ==> AJ



J

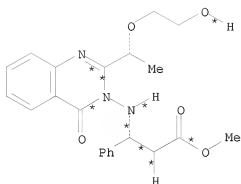


AD



AA

5
STEPS
→



AJ

YIELD 95%

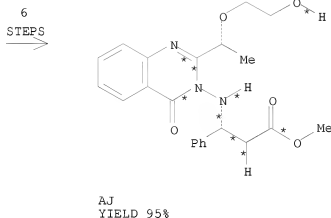
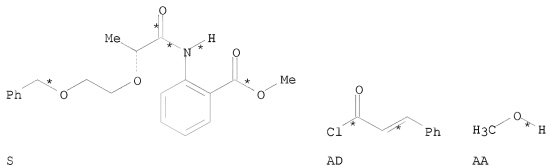
RX(4)	RCT	J 445397-15-9
	RGT	L 302-01-2 N2H4
	PRO	K 445397-14-8
	SOL	64-17-5 EtOH
RX(8)	RCT	K 445397-14-8, AD 17082-09-6
	RGT	Z 110-86-1 Pyridine
	PRO	AE 445397-17-1
	SOL	75-09-2 CH2Cl2
RX(9)	RCT	AE 445397-17-1
	RGT	C 546-67-8 Pb(OAc)4, D 999-97-3 (Me3Si)2NH
	PRO	AF 445397-18-2
	SOL	75-09-2 CH2Cl2
	NTE	stereoselective
RX(10)	RCT	AF 445397-18-2
	RGT	AH 32248-43-4 SmI2
	PRO	AG 445397-19-3

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SOL 109-99-9 THF, 75-65-0 t-BuOH

RX(11) RCT AG 445397-19-3, AA 67-56-1
 RGT X 124-41-4 NaOMe
 PRO AJ 445397-20-6
 SOL 67-56-1 MeOH

RX(42) OF 54 COMPOSED OF RX(6), RX(4), RX(8), RX(9), RX(10), RX(11)
 RX(42) S + AD + AA ==> AJ



RX(6) RCT S 445397-16-0
 RGT T 1333-74-0 H2
 PRO J 445397-15-9
 CAT 7440-05-3 Pd
 SOL 64-19-7 AcOH

RX(4) RCT J 445397-15-9
 RGT L 302-01-2 N2H4
 PRO K 445397-14-8
 SOL 64-17-5 EtOH

RX(8) RCT K 445397-14-8, AD 17082-09-6
 RGT Z 110-86-1 Pyridine
 PRO AE 445397-17-1

10/ 562,112

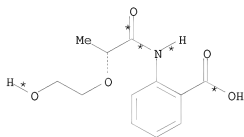
SOL 75-09-2 CH2Cl2

RX(9) RCT AE 445397-17-1
RGT C 546-67-8 Pb(OAc)4, D 999-97-3 (Me3Si)2NH
PRO AF 445397-18-2
SOL 75-09-2 CH2Cl2
NTE stereoselective

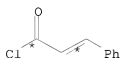
RX(10) RCT AF 445397-18-2
RGT AH 32248-43-4 SmI2
PRO AG 445397-19-3
SOL 109-99-9 THF, 75-65-0 t-BuOH

RX(11) RCT AG 445397-19-3, AA 67-56-1
RGT X 124-41-4 NaOMe
PRO AJ 445397-20-6
SOL 67-56-1 MeOH

RX(51) OF 54 COMPOSED OF RX(4), RX(8), RX(9), RX(10), RX(11), RX(12)
RX(51) J + AD + AA ==> AK + AL



J

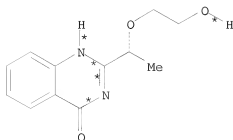


AD

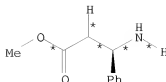


AA

6
STEPS
→



AK



AL

RX(4) RCT J 445397-15-9
RGT L 302-01-2 N2H4

PRO K 445397-14-8
 SOL 64-17-5 EtOH

RX(8) RCT K 445397-14-8, AD 17082-09-6
 RGT Z 110-86-1 Pyridine
 PRO AE 445397-17-1
 SOL 75-09-2 CH₂Cl₂

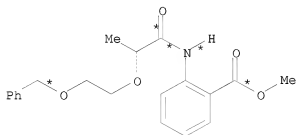
RX(9) RCT AE 445397-17-1
 RGT C 546-67-8 Pb(OAc)₄, D 999-97-3 (Me₃Si)₂NH
 PRO AF 445397-18-2
 SOL 75-09-2 CH₂Cl₂
 NTE stereoselective

RX(10) RCT AF 445397-18-2
 RGT AH 32248-43-4 SmI₂
 PRO AG 445397-19-3
 SOL 109-99-9 THF, 75-65-0 t-BuOH

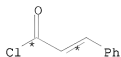
RX(11) RCT AG 445397-19-3, AA 67-56-1
 RGT X 124-41-4 NaOMe
 PRO AJ 445397-20-6
 SOL 67-56-1 MeOH

RX(12) RCT AJ 445397-20-6
 RGT AH 32248-43-4 SmI₂, AM 108-01-0 Me₂NCH₂CH₂OH
 PRO AK 445397-21-7, AL 37088-67-8
 SOL 109-99-9 THF
 NTE 40% overall yield

RX(52) OF 54 COMPOSED OF RX(6), RX(4), RX(8), RX(9), RX(10), RX(11), RX(12)
 RX(52) S + AD + AA ==> AK + AL



S

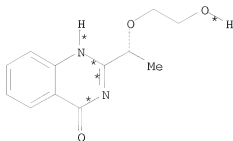


AD

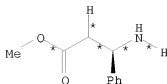


AA

7
STEPS
→



AK



AL

RX(6)	RCT	S 445397-16-0
	RGT	T 1333-74-0 H2
	PRO	J 445397-15-9
	CAT	7440-05-3 Pd
	SOL	64-19-7 AcOH
RX(4)	RCT	J 445397-15-9
	RGT	L 302-01-2 N2H4
	PRO	K 445397-14-8
	SOL	64-17-5 EtOH
RX(8)	RCT	K 445397-14-8, AD 17082-09-6
	RGT	Z 110-86-1 Pyridine
	PRO	AE 445397-17-1
	SOL	75-09-2 CH2Cl2
RX(9)	RCT	AE 445397-17-1
	RGT	C 546-67-8 Pb(OAc)4, D 999-97-3 (Me3Si)2NH
	PRO	AF 445397-18-2
	SOL	75-09-2 CH2Cl2
	NTE	stereoselective
RX(10)	RCT	AF 445397-18-2
	RGT	AH 32248-43-4 SmI2
	PRO	AG 445397-19-3
	SOL	109-99-9 THF, 75-65-0 t-BuOH
RX(11)	RCT	AG 445397-19-3, AA 67-56-1
	RGT	X 124-41-4 NaOMe
	PRO	AJ 445397-20-6
	SOL	67-56-1 MeOH
RX(12)	RCT	AJ 445397-20-6
	RGT	AH 32248-43-4 SmI2, AM 108-01-0 Me2NCH2CH2OH
	PRO	AK 445397-21-7, AL 37088-67-8
	SOL	109-99-9 THF
	NTE	40% overall yield

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 99 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 137:47172 CASREACT

TITLE: Di-4(3H)-quinazolinon-2-yl derivatives from the diacid chlorides of pinic and sym-homopinic acids

AUTHOR(S): Avotin'sh, F. M.; Petrova, M. V.; Strakov, A. Ya.

CORPORATE SOURCE: Riga Technical University, Riga, LV-1658, Latvia

SOURCE: Chemistry of Heterocyclic Compounds (New York, NY, United States)(Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2001), 37(10), 1241-1243

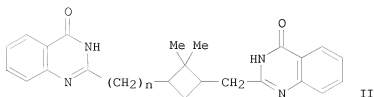
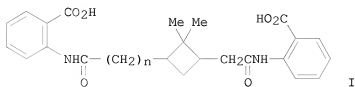
CODEN: CHCCAL; ISSN: 0009-3122

PUBLISHER: Kluwer Academic/Consultants Bureau

DOCUMENT TYPE: Journal

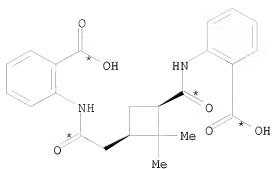
LANGUAGE: English

GI



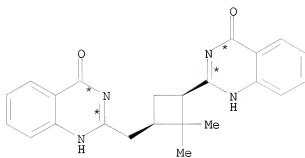
AB The corresponding dianthranilamides I ($n = 0, 1$) were synthesized by the interaction of the diacid chlorides of *cis*-2,2-dimethyl-3-carboxycyclobutaneacetic acid (pinic acid) and *cis*-2,2-dimethylcyclobutane-1,3-diacetic acid (sym-homopinic acid) with two equivalent of anthranilic acid. Treatment of the dianthranilamides with formamide gave 2,2-dimethyl-1-[4(3H)-quinazolinon-2-yl]methyl-3-[4(3H)-quinazolinon-2-yl]cyclobutane II ($n = 0$) and 2,2-dimethyl-1,3-di[4(3H)-quinazolinon-2-ylmethyl]cyclobutane II ($n = 1$), resp.

RX(3) OF 8 ...C ==> H



C

(3) →

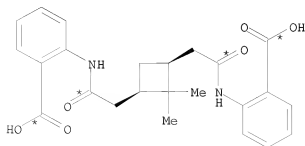


H

YIELD 69%

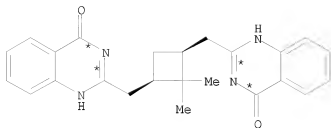
RX(3) RCT C 438001-74-2
 PRO H 438001-76-4
 SOL 75-12-7 Formamide
 NTE thermal

RX(4) OF 8 ...G ==> J



G

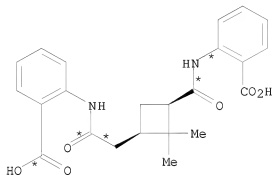
(4) →



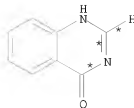
J
YIELD 65%

RX(4) RCT G 438001-75-3
PRO J 438001-77-5
SOL 75-12-7 Formamide
NTE thermal

RX(5) OF 8 ...C ==> K



C



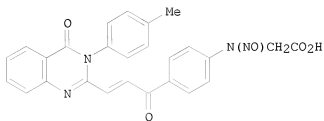
K
YIELD 20%

RX(5) RCT C 438001-74-2
RGT L 7647-01-0 HCl
PRO K 491-36-1
SOL 7732-18-5 Water

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 100 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 136:294792 CASREACT
TITLE: Synthesis and antimicrobial evaluation of chalcone and sydnone derivatives of 4(3H)-quinazolinone
AUTHOR(S): Bekhit, Adnan A.; Habib, Nargues S.; Bekhit, El-Din A.
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Alexandria, Alexandria, Egypt

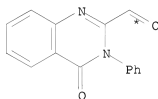
SOURCE: Bollettino Chimico Farmaceutico (2001), 140(5), 297-301
 CODEN: BCFAAI; ISSN: 0006-6648
 PUBLISHER: Societa Editoriale Farmaceutica
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



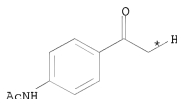
I

AB The increasing clin. importance of drug-resistant bacterial pathogens has encouraged addnl. microbiol. and antibacterial research. New chalcone and sydnone derivs. of 4(3H)-quinazolinone were synthesized and evaluated for their antibacterial and antifungal activity. The microorganisms used were Escherichia coli ATCC 25922 as Gram-neg. bacteria, Staphylococcus aureus ATCC 19433 as Gram-Pos. bacteria and Candida albicans as yeast-like fungi. The most potent compound was the nitroso derivative I.

RX(1) OF 21 A + B ==> C

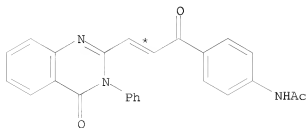


A



B

(1) →



C
 YIELD 82%

RX(1) RCT A 20873-11-4, B 2719-21-3

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STAGE(1)

RGT D 1310-73-2 NaOH

SOL 64-17-5 EtOH

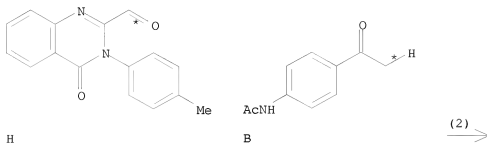
STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO C 407631-31-6

RX(2) OF 21 H + B ==> I



I
YIELD 76%

RX(2) RCT H 53678-82-3, B 2719-21-3

STAGE(1)

RGT D 1310-73-2 NaOH

SOL 64-17-5 EtOH

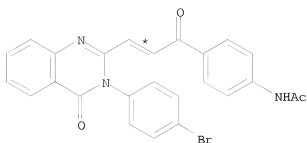
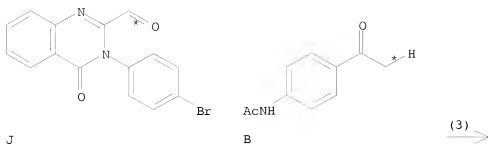
STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO I 407631-32-7

RX(3) OF 21 J + B ==> K



YIELD 87%

RX(3) RCT J 131532-68-8, B 2719-21-3

STAGE(1)

RGT D 1310-73-2 NaOH
SOL 64-17-5 EtOH

STAGE(2)

RGT E 7647-01-0 HCl
SOL 7732-18-5 Water

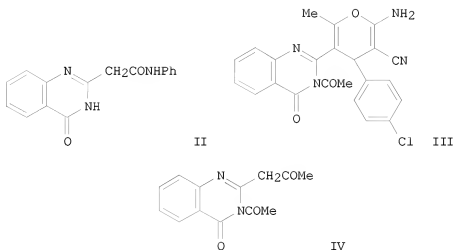
PRO K 407631-33-8

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 101 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 136:247541 CASREACT
 TITLE: A new route for the synthesis of some quinazoline derivatives
 AUTHOR(S): Youssef, A. M. S.; Faty, Rasha A. M.
 CORPORATE SOURCE: Chemistry Department, Faculty of Science, Fayoum Branch, Cairo University, Fayoum, Egypt
 SOURCE: Egyptian Journal of Chemistry (2001), 44(4-6), 227-235
 CODEN: EGJCA3; ISSN: 0449-2285
 PUBLISHER: National Information and Documentation Centre
 DOCUMENT TYPE: Journal

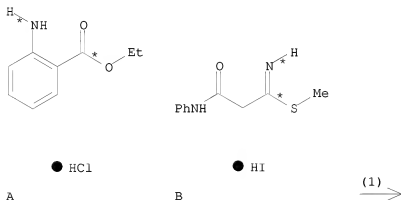
LANGUAGE:
GI

English

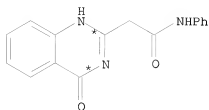


AB S-Me monothiomalonanilide hydroiodide (I) is a versatile compound for synthesizing quinazoline derivs. Thus, I reacted with either anthranilic acid or Et anthranilate hydrochloride to yield II. Also, polysubstituted pyranylquinazolinone III was obtained by reaction of quinazolinone derivative IV with p-chloro- α -cyanocinnamionitrile. Chemical and spectroscopic evidence for the structures of the newly synthesized compds. are described.

RX(1) OF 30 A + B ==> C...



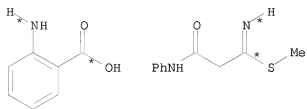
10/ 562,112



C
YIELD 65%

RX(1) RCT A 32045-49-1, B 59750-09-3
RGT D 127-09-3 AcONa
PRO C 74089-31-9
SOL 64-17-5 EtOH

RX(2) OF 30 F + B ==> C...

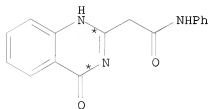


F

B

● HI

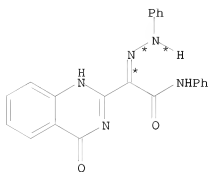
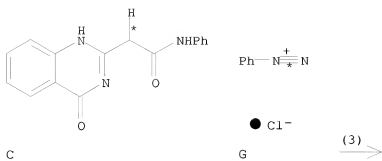
(2) ➔



C

RX(2) RCT F 118-92-3, B 59750-09-3
PRO C 74089-31-9
SOL 64-17-5 EtOH

RX(3) OF 30 ...C + G ==> H



H
YIELD 55%

RX(3) RCT C 74089-31-9

STAGE(1)

RGT D 127-09-3 AcONa

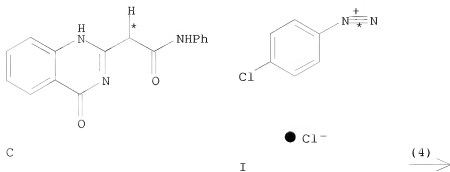
SOL 64-17-5 EtOH

STAGE(2)

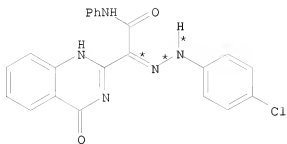
RCT G 100-34-5

PRO H 404384-07-2

RX(4) OF 30 ...C + I \implies J



10/ 562,112



J
YIELD 57%

RX(4) RCT C 74089-31-9

STAGE(1)

RGT D 127-09-3 AcONa

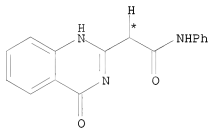
SOL 64-17-5 EtOH

STAGE(2)

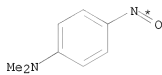
RCT I 2028-74-2

PRO J 404384-08-3

RX(5) OF 30 ...C + K ==> L

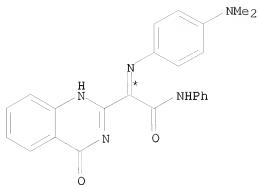


C



K

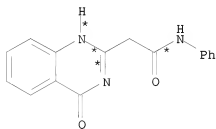
(5)
→



L
YIELD 40%

RX(5) RCT C 74089-31-9, K 138-89-6
RGT D 127-09-3 AcONa
PRO L 404384-09-4
CAT 110-89-4 Piperidine
SOL 64-17-5 EtOH

RX(6) OF 30 ...C + N ==> O...

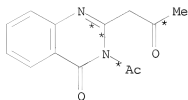


C



N

(6) →



O
YIELD 69%

RX(6) RCT C 74089-31-9, N 108-24-7

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STAGE(1)

SOL 108-24-7 Ac2O

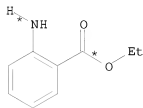
STAGE(2)

RGT P 7732-18-5 Water

PRO O 404384-10-7

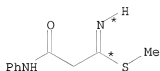
RX(11) OF 30 COMPOSED OF RX(1), RX(3)

RX(11) A + B + G ==> H



● HCl

A



● HI

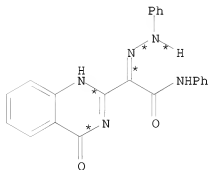
B



● Cl⁻

G

2
STEPS
➔



H
YIELD 55%

RX(1) RCT A 32045-49-1, B 59750-09-3

RGT D 127-09-3 AcONa

PRO C 74089-31-9

SOL 64-17-5 EtOH

RX(3) RCT C 74089-31-9

STAGE(1)

RGT D 127-09-3 AcONa

SOL 64-17-5 EtOH

10/ 562,112

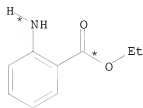
STAGE(2)

RCT G 100-34-5

PRO H 404384-07-2

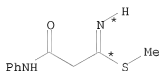
RX(12) OF 30 COMPOSED OF RX(1), RX(4)

RX(12) A + B + I ==> J



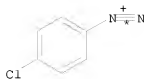
● HCl

A



● HI

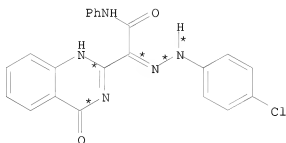
B



● Cl⁻

I

2
STEPS
→



J
YIELD 57%

RX(1) RCT A 32045-49-1, B 59750-09-3

RGT D 127-09-3 AcONa

PRO C 74089-31-9

SOL 64-17-5 EtOH

RX(4) RCT C 74089-31-9

STAGE(1)

RGT D 127-09-3 AcONa

SOL 64-17-5 EtOH

STAGE(2)

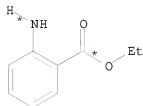
10/ 562,112

RCT I 2028-74-2

PRO J 404384-08-3

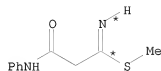
RX(13) OF 30 COMPOSED OF RX(1), RX(5)

RX(13) A + B + K ==> L



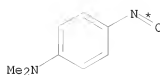
● HCl

A



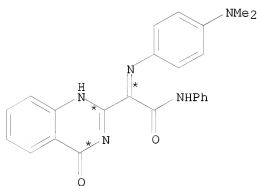
● HI

B



K

2
STEPS
→



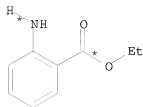
L
YIELD 40%

RX(1) RCT A 32045-49-1, B 59750-09-3
RGT D 127-09-3 AcONa
PRO C 74089-31-9
SOL 64-17-5 EtOH

RX(5) RCT C 74089-31-9, K 138-89-6
RGT D 127-09-3 AcONa
PRO L 404384-09-4
CAT 110-89-4 Piperidine
SOL 64-17-5 EtOH

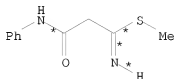
10/ 562,112

RX(14) OF 30 COMPOSED OF RX(1), RX(6)
 RX(14) A + B + N ==> O



● HCl

A



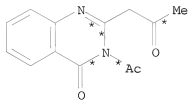
● HI

B



N

2
 STEPS
 →



O
 YIELD 69%

RX(1) RCT A 32045-49-1, B 59750-09-3
 RGT D 127-09-3 AcONa
 PRO C 74089-31-9
 SOL 64-17-5 EtOH

RX(6) RCT C 74089-31-9, N 108-24-7

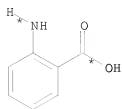
STAGE(1)
 SOL 108-24-7 Ac2O

STAGE(2)
 RGT P 7732-18-5 Water

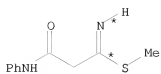
PRO O 404384-10-7

RX(15) OF 30 COMPOSED OF RX(2), RX(3)
 RX(15) F + B + G ==> H

10/ 562,112



F

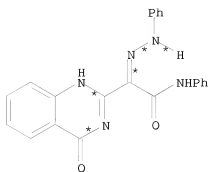


B



G

2
STEPS
→



H
YIELD 55%

RX(2) RCT F 118-92-3, B 59750-09-3
PRO C 74089-31-9
SOL 64-17-5 EtOH

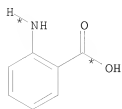
RX(3) RCT C 74089-31-9

STAGE(1)
RGT D 127-09-3 AcONa
SOL 64-17-5 EtOH

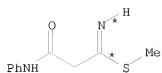
STAGE(2)
RCT G 100-34-5

PRO H 404384-07-2

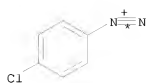
RX(16) OF 30 COMPOSED OF RX(2), RX(4)
RX(16) F + B + I ==> J



F

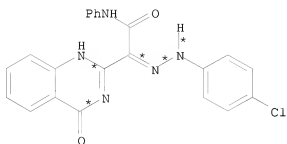


B



I

2
STEPS
→



J

YIELD 57%

RX(2) RCT F 118-92-3, B 59750-09-3
PRO C 74089-31-9
SOL 64-17-5 EtOH

RX(4) RCT C 74089-31-9

STAGE(1)

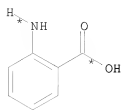
RGT D 127-09-3 AcONa
SOL 64-17-5 EtOH

STAGE(2)

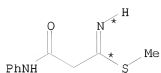
RCT I 2028-74-2

PRO J 404384-08-3

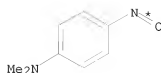
RX(17) OF 30 COMPOSED OF RX(2), RX(5)
RX(17) F + B + K ==> L



F

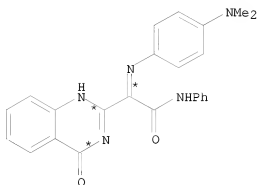


B



K

2
STEPS
→



L

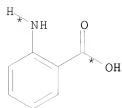
YIELD 40%

RX(2) RCT F 118-92-3, B 59750-09-3
PRO C 74089-31-9
SOL 64-17-5 EtOH

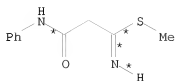
RX(5) RCT C 74089-31-9, K 138-89-6
RGT D 127-09-3 AcONa
PRO L 404384-09-4
CAT 110-89-4 Piperidine
SOL 64-17-5 EtOH

RX(18) OF 30 COMPOSED OF RX(2), RX(6)
RX(18) F + B + N ==> O

10/ 562,112



F



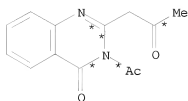
B

● HI



N

2
STEPS
→



O

YIELD 69%

RX(2) RCT F 118-92-3, B 59750-09-3
PRO C 74089-31-9
SOL 64-17-5 EtOH

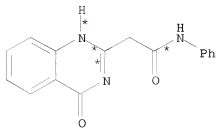
RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)
SOL 108-24-7 Ac2O

STAGE(2)
RGT P 7732-18-5 Water

PRO O 404384-10-7

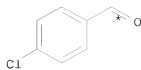
RX(19) OF 30 COMPOSED OF RX(6), RX(8)
RX(19) C + N + T ==> U



C



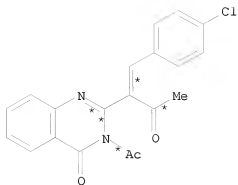
N



T

10/ 562,112

2
STEPS
→



U
YIELD 35%

RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)

SOL 108-24-7 Ac2O

STAGE(2)

RGT P 7732-18-5 Water

PRO O 404384-10-7

RX(8) RCT O 404384-10-7, T 104-88-1

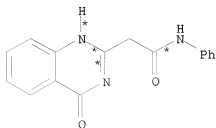
RGT D 127-09-3 AcONa

PRO U 404384-11-8

SOL 64-19-7 AcOH

RX(20) OF 30 COMPOSED OF RX(6), RX(9)

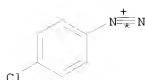
RX(20) C + N + I ==> W



C



N

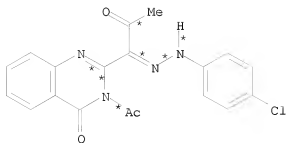


● Cl⁻

I

10/ 562,112

2
STEPS
→



W
YIELD 63%

RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)

SOL 108-24-7 Ac2O

STAGE(2)

RGT P 7732-18-5 Water

PRO O 404384-10-7

RX(9) RCT O 404384-10-7

STAGE(1)

RGT D 127-09-3 AcONa

SOL 64-17-5 EtOH

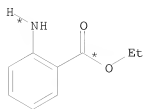
STAGE(2)

RCT I 2028-74-2

PRO W 404384-12-9

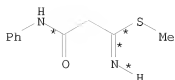
RX(25) OF 30 COMPOSED OF RX(1), RX(6), RX(8)

RX(25) A + B + N + T ==> U



● HCl

A

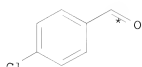


● HI

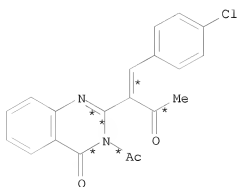
B



N



T

3
STEPS
→U
YIELD 35%

RX(1) RCT A 32045-49-1, B 59750-09-3
RGT D 127-09-3 AcONa
PRO C 74089-31-9
SOL 64-17-5 EtOH

RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)
SOL 108-24-7 Ac2O

STAGE(2)
RGT P 7732-18-5 Water

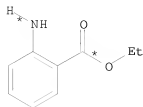
PRO O 404384-10-7

RX(8) RCT O 404384-10-7, T 104-88-1
RGT D 127-09-3 AcONa
PRO U 404384-11-8
SOL 64-19-7 AcOH

RX(26) OF 30 COMPOSED OF RX(1), RX(6), RX(9)

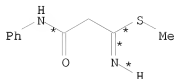
10/ 562,112

RX(26) A + B + N + I ==> W



● HCl

A

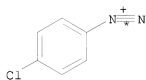


● HI

B



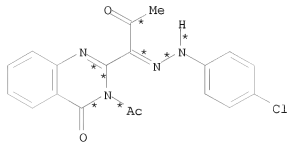
N



● Cl⁻

I

3
STEPS
→



W
YIELD 63%

RX(1) RCT A 32045-49-1, B 59750-09-3
 RGT D 127-09-3 AcONa
 PRO C 74089-31-9
 SOL 64-17-5 EtOH

RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)
 SOL 108-24-7 Ac2O

STAGE(2)
 RGT P 7732-18-5 Water

PRO O 404384-10-7

RX(9) RCT O 404384-10-7

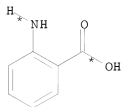
STAGE(1)
 RGT D 127-09-3 AcONa
 SOL 64-17-5 EtOH

STAGE(2)
 RCT I 2028-74-2

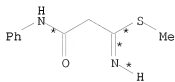
10/ 562,112

PRO W 404384-12-9

RX(28) OF 30 COMPOSED OF RX(2), RX(6), RX(8)
 RX(28) F + B + N + T ==> U



F

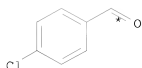


B

● HI

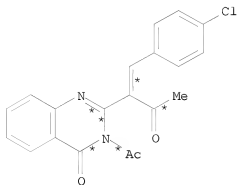


N



T

3
STEPS
→



U

YIELD 35%

RX(2) RCT F 118-92-3, B 59750-09-3
 PRO C 74089-31-9
 SOL 64-17-5 EtOH

RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)
 SOL 108-24-7 Ac2O

STAGE(2)

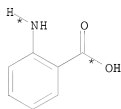
RGT P 7732-18-5 Water

PRO O 404384-10-7

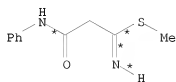
RX(8) RCT O 404384-10-7, T 104-88-1
 RGT D 127-09-3 AcONa
 PRO U 404384-11-8
 SOL 64-19-7 AcOH

RX(29) OF 30 COMPOSED OF RX(2), RX(6), RX(9)

RX(29) F + B + N + I ==> W

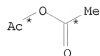


F

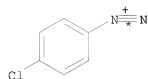


B

● HI

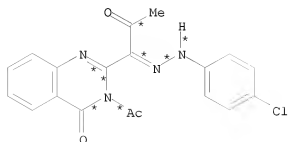


N

● Cl⁻

I

3
 STEPS
 →



W
 YIELD 63%

RX(2) RCT F 118-92-3, B 59750-09-3
 PRO C 74089-31-9
 SOL 64-17-5 EtOH

RX(6) RCT C 74089-31-9, N 108-24-7

STAGE(1)

SOL 108-24-7 Ac2O

STAGE(2)

RGT P 7732-18-5 Water

PRO O 404384-10-7

RX(9) RCT O 404384-10-7

STAGE(1)

RGT D 127-09-3 AcONa

SOL 64-17-5 EtOH

STAGE(2)

RCT I 2028-74-2

PRO W 404384-12-9

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 102 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 136:118618 CASREACT

TITLE: Concise and Efficient Synthesis of Bioactive Natural Products Pegamine, Deoxyvasicinone, and (-)-Vasicinone

AUTHOR(S): Mhaske, Santosh B.; Argade, Narshinha P.

CORPORATE SOURCE: Division of Organic Chemistry (Synthesis), National Chemical Laboratory, Pune, 411 008, India

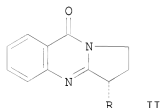
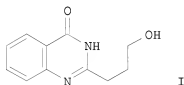
SOURCE: Journal of Organic Chemistry (2001), 66(26), 9038-9040
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

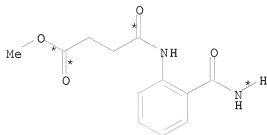


AB The authors have demonstrated a most concise, efficient, and practical synthesis of naturally occurring bioactive quinazolinone alkaloids pegamine (I), deoxyvasicinone (II, R = H), (-)-vasicinone (II, R = OH), for the first time starting from succinic anhydride and (S)-acetoxysuccinic anhydride. A formal synthesis of rutecarpine, isaindigotone, and luotonins A and B has been implied. The present approach also provides a new general method for designing several quinazolinone derivs. using a variety of cyclic anhydrides for structure

10/ 562,112

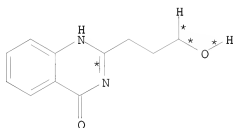
activity relationship studies.

RX(4) OF 32 ...M ==> A...



M

(4)



A

YIELD 93%

RX(4) RCT M 105234-41-1

STAGE(1)

RGT O 16853-85-3 LiAlH₄

SOL 109-99-9 THF

STAGE(2)

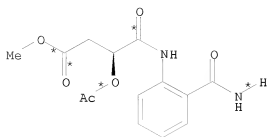
RGT P 7732-18-5 Water

PRO A 31431-93-3

NTE chemoselective

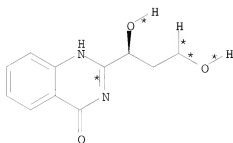
RX(8) OF 32 ...U ==> V...

10/ 562,112



U

(8) \Rightarrow



V

YIELD 92%

RX(8) RCT U 391249-54-0

STAGE(1)

RGT O 16853-85-3 LiAlH₄

SOL 109-99-9 THF

STAGE(2)

RGT P 7732-18-5 Water

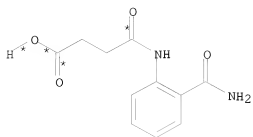
PRO V 391249-56-2

NTE stereoselective, chemoselective

RX(13) OF 32 COMPOSED OF RX(3), RX(4)

RX(13) H + L \Rightarrow A

10/ 562,112

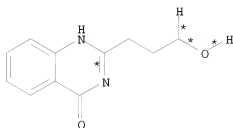


H



L

2
STEPS
→



A

YIELD 93%

RX(3) RCT H 306325-56-4, L 334-88-3

STAGE(1)

SOL 60-29-7 Et2O

STAGE(2)

RGT N 64-19-7 AcOH

PRO M 105234-41-1

RX(4) RCT M 105234-41-1

STAGE(1)

RGT O 16853-85-3 LiAlH4

SOL 109-99-9 THF

STAGE(2)

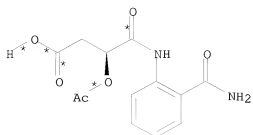
RGT P 7732-18-5 Water

PRO A 31431-93-3

NIE chemoselective

RX(17) OF 32 COMPOSED OF RX(7), RX(8)

RX(17) T + L ==> V

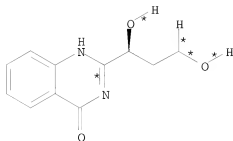


T



L

2
STEPS
→



V

YIELD 92%

RX(7) RCT T 391249-53-9, L 334-88-3

STAGE(1)

SOL 60-29-7 Et2O

STAGE(2)

RGT N 64-19-7 AcOH

PRO U 391249-54-0

NTE stereoselective

RX(8) RCT U 391249-54-0

STAGE(1)

RGT O 16853-85-3 LiAlH4

SOL 109-99-9 THF

STAGE(2)

RGT P 7732-18-5 Water

PRO V 391249-56-2

NTE stereoselective, chemoselective

REFERENCE COUNT:

64

THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 103 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 135:152997 CASREACT
 TITLE: Synthesis of ent-Alantrypinone
 AUTHOR(S): Hart, David J.; Magomedov, Nabi A.
 CORPORATE SOURCE: Department of Chemistry, The Ohio State University,
 Columbus, OH, 43210, USA
 SOURCE: Journal of the American Chemical Society (2001),
 123(25), 5892-5899
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

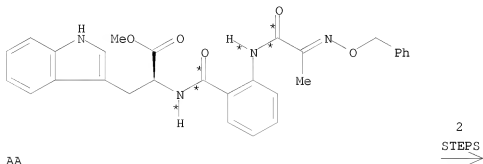
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB This paper presents a synthesis of ent-alantrypinone, the enantiomer of a natural product produced by the fungus *Penicillium thymicola*. The synthesis revolves around the Li[Me₃AlSPH]-promoted isomerization of iminobenzoxazine I to quinazolinone II, an N-acyliminium ion cyclization that converts enamide III to bridged indole, and rearrangement to oxindole title product. Ancillary chemical that involves thermal fragmentation of an iminobenzoxazine to a nitrile ylide and Me₂AlSPH-mediated cyclization of oxime ether-ester to pyrrolidinone is also described.

```

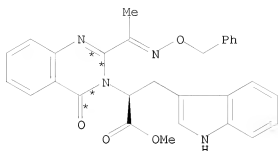
RX(39) OF 179 COMPOSED OF RX(11), RX(1)
RX(39)      AA  ==>  B

```



AA

10/ 562,112



B

YIELD 90%

RX(11) RCT AA 352665-14-6
 RGT M 603-35-0 PPh3, AG 7553-56-2 I2, AH 7087-68-5 EtN(Pr-i)2
 PRO A 352665-17-9
 SOL 75-09-2 CH2Cl2

RX(1) RCT A 352665-17-9

STAGE(1)

RGT C 108-98-5 PhSH, D 109-72-8 BuLi

SOL 75-09-2 CH2Cl2, 108-88-3 PhMe, 110-54-3 Hexane

STAGE(2)

SOL 75-09-2 CH2Cl2

STAGE(3)

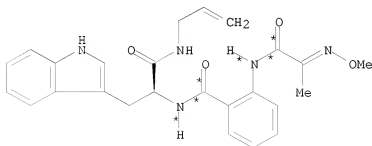
RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO B 352665-10-2

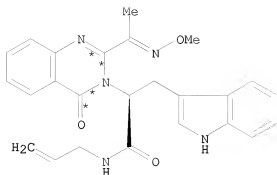
RX(42) OF 179 COMPOSED OF RX(16), RX(17)

RX(42) AR ==> AU



2
 STEPS
 →

AR



AU
YIELD 93%

RX(16) RCT AR 352665-20-4
RGT M 603-35-0 PPh3, AG 7553-56-2 I2, AH 7087-68-5 EtN(Pr-i)2
PRO AS 352665-21-5
SOL 75-09-2 CH2Cl2, 109-99-9 THF

RX(17) RCT AS 352665-21-5

STAGE(1)

RGT C 108-98-5 PhSH, D 109-72-8 BuLi
SOL 75-09-2 CH2Cl2, 108-88-3 PhMe, 110-54-3 Hexane

STAGE(2)

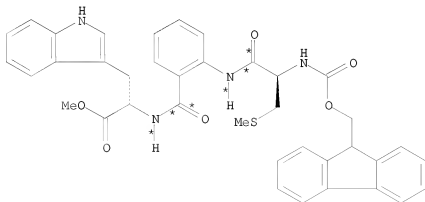
SOL 75-09-2 CH2Cl2

STAGE(3)

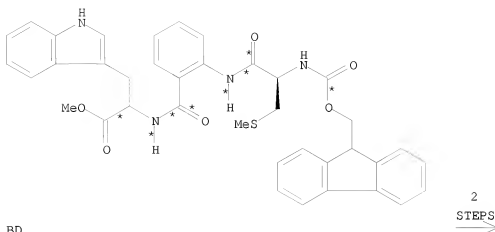
RGT E 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AU 352665-22-6

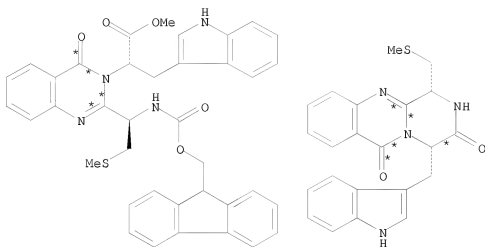
RX(50) OF 179 COMPOSED OF RX(22), RX(23)
RX(50) 2 BD ==> AV + J



BD



BD



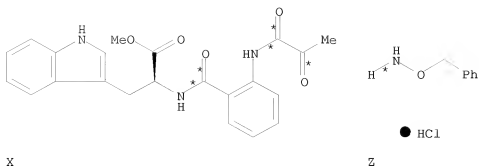
AV
YIELD 76%

J
YIELD 8%

RX(22) RCT BD 246848-99-7
RGT M 603-35-0 PPh3, AG 7553-56-2 I2, AH 7087-68-5 EtN(Pr-i)2
PRO BF 246849-00-3
SOL 75-09-2 CH2Cl2

RX(23) RCT BF 246849-00-3
RGT C 108-98-5 PhSH, D 109-72-8 BuLi, V 75-24-1 AlMe3
PRO AV 246849-02-5, J 246849-03-6
SOL 109-99-9 THF, 110-54-3 Hexane, 108-88-3 PhMe

RX(72) OF 179 COMPOSED OF RX(7), RX(11), RX(1)
RX(72) X + Z ==> B



RX(7) RCT X 352665-12-4, Z 2687-43-6
 RGT AB 110-86-1 Pyridine
 PRO AA 352665-14-6
 SOL 67-56-1 MeOH

RX(11) RCT AA 352665-14-6
 RGT M 603-35-0 PPh3, AG 7553-56-2 I2, AH 7087-68-5 EtN(Pr-i)2
 PRO A 352665-17-9
 SOL 75-09-2 CH2Cl2

RX(1) RCT A 352665-17-9

STAGE(1)

RGT C 108-98-5 PhSH, D 109-72-8 BuLi
 SOL 75-09-2 CH2Cl2, 108-88-3 PhMe, 110-54-3 Hexane

STAGE(2)

SOL 75-09-2 CH2Cl2

STAGE(3)

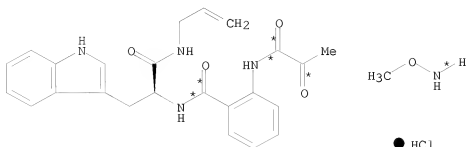
RGT E 7647-01-0 HCl
 SOL 7732-18-5 Water

PRO B 352665-10-2

RX(74) OF 179 COMPOSED OF RX(15), RX(16), RX(17)

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RX(74) Y + AQ ==> AU

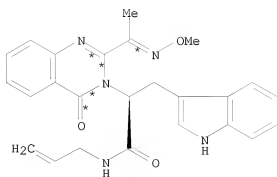


Y

● HCl

AQ

3
STEPS
→



AU

YIELD 93%

RX(15) RCT Y 352665-13-5, AQ 593-56-6
 RGT AB 110-86-1 Pyridine
 PRO AR 352665-20-4
 SOL 67-56-1 MeOH

RX(16) RCT AR 352665-20-4
 RGT M 603-35-0 PPh3, AG 7553-56-2 I2, AH 7087-68-5 EtN(Pr-i)2
 PRO AS 352665-21-5
 SOL 75-09-2 CH2Cl2, 109-99-9 THF

RX(17) RCT AS 352665-21-5

STAGE(1)

RGT C 108-98-5 PhSH, D 109-72-8 BuLi
SOL 75-09-2 CH2Cl2, 108-88-3 PhMe, 110-54-3 Hexane

STAGE(2)

SOL 75-09-2 CH2Cl2

STAGE(3)

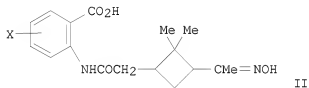
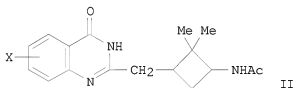
RGT E 7647-01-0 HC1

SOL 7732-18-5 Water

PRO AU 352665-22-6

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

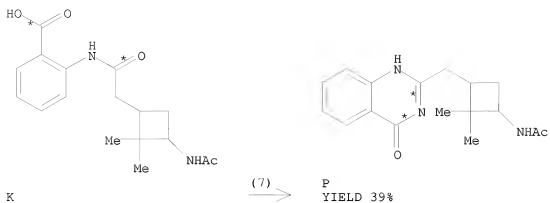
L3 ANSWER 104 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 135:137461 CASREACT
 TITLE: 2-[(3-Acetylamino-2,2-dimethylcyclobutyl)methyl]-4(3H)-quinazolinones
 AUTHOR(S): Avotin'sh, F. M.; Petrova, M. V.; Tonkikh, N. N.; Strakov, A.
 CORPORATE SOURCE: Riga Technical University, Riga, LV-1658, Latvia
 SOURCE: Chemistry of Heterocyclic Compounds (New York, NY, United States)(Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2000), 36(11), 1326-1328
 CODEN: CHCCAL; ISSN: 0009-3122
 CONSULTANTS BUREAU
 PUBLISHER: Journal
 DOCUMENT TYPE: English
 LANGUAGE: English
 GI



AB The title compds. (I; X = H, 6-Br, 7-Cl) were prepared by Beckmann rearrangement of oximes II (X = 5-Br, 4-Cl), followed by cyclization with formamide.

RX(7) OF 18 ...K ==> P

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RX(7) RCT K 259262-89-0

STAGE(1)

RGT Q 75-12-7 Formamide

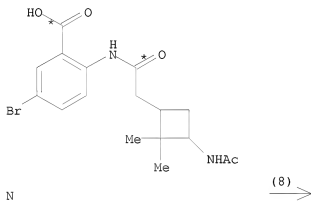
STAGE(2)

RGT R 144-55-8 NaHCO₃

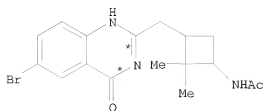
SOL 7732-18-5 Water

PRO P 352031-50-6

RX(8) OF 18 ...N ==> S



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S
YIELD 41%

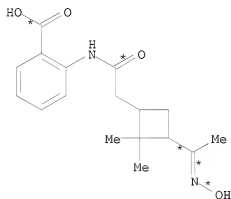
RX(8) RCT N 352031-48-2

STAGE(1)
RGT Q 75-12-7 Formamide

STAGE(2)
RGT R 144-55-8 NaHCO3
SOL 7732-18-5 Water

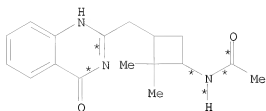
PRO S 352031-51-7

RX(13) OF 18 COMPOSED OF RX(4), RX(7)
RX(13) B ==> P



B

2
STEPS
→



P
YIELD 39%

RX(4) RCT B 259262-88-9

STAGE(1)

STAGE(2)

RGT L 1336-21-6 NH₄OH

SOL 7732-18-5 Water

STAGE(3)

SOL 141-78-6 AcOEt

PRO K 259262-89-0

NTE polyphosphoric acid used in first stage

RX(7) RCT K 259262-89-0

STAGE(1)

RGT Q 75-12-7 Formamide

STAGE(2)

RGT R 144-55-8 NaHCO₃

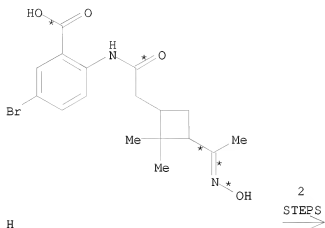
SOL 7732-18-5 Water

PRO P 352031-50-6

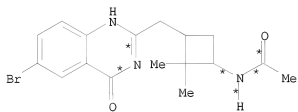
RX(14) OF 18 COMPOSED OF RX(5), RX(8)

RX(14) H ==> S

10/ 562,112



H



S

YIELD 41%

RX(5) RCT H 352031-46-0

STAGE(1)

STAGE(2)

RGT L 1336-21-6 NH4OH

SOL 7732-18-5 Water

STAGE(3)

SOL 141-78-6 AcOEt

PRO N 352031-48-2

RX(8) RCT N 352031-48-2

STAGE(1)

RGT Q 75-12-7 Formamide

STAGE(2)

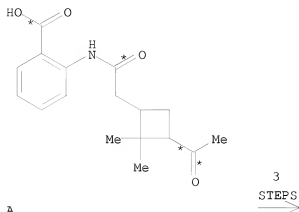
RGT R 144-55-8 NaHCO3

SOL 7732-18-5 Water

PRO S 352031-51-7

10/ 562,112

RX(16) OF 18 COMPOSED OF RX(1), RX(4), RX(7)
RX(16) A ==> P



P
YIELD 39%

RX(1) RCT A 259262-85-6

STAGE(1)

RGT C 5470-11-1 H2NOH-HCl, D 127-09-3 AcONa
SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO B 259262-88-9

RX(4) RCT B 259262-88-9

STAGE(1)

STAGE(2)

RGT L 1336-21-6 NH4OH
SOL 7732-18-5 Water

STAGE(3)

SOL 141-78-6 AcOEt

PRO K 259262-89-0

NTE polyphosphoric acid used in first stage

10/ 562,112

RX(7) RCT K 259262-89-0

STAGE(1)

RGT Q 75-12-7 Formamide

STAGE(2)

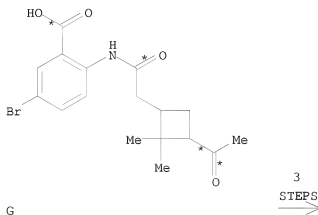
RGT R 144-55-8 NaHCO3

SOL 7732-18-5 Water

PRO P 352031-50-6

RX(17) OF 18 COMPOSED OF RX(2), RX(5), RX(8)

RX(17) G ==> S



S
YIELD 41%

RX(2) RCT G 259262-86-7

STAGE(1)

RGT C 5470-11-1 H2NOH-HCl, D 127-09-3 AcONa

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO H 352031-46-0

RX(5) RCT H 352031-46-0

STAGE(1)

STAGE(2)
RGT L 1336-21-6 NH4OH
SOL 7732-18-5 Water

STAGE(3)
SOL 141-78-6 AcOEt

PRO N 352031-48-2

RX(8) RCT N 352031-48-2

STAGE(1)
RGT Q 75-12-7 Formamide

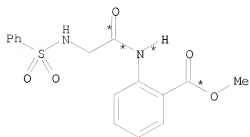
STAGE(2)
RGT R 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO S 352031-51-7

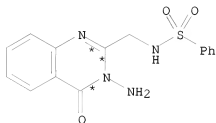
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 105 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 135:122713 CASREACT
TITLE: Amino acids in the synthesis of heterocyclic systems:
The synthesis of triazinoquinazolinones,
triazepinoquinazolinones and triazocinoquinazolinones
of potential biological interest
AUTHOR(S): El-Sharief, A. M. Sh.; Ammar, Y. A.; Zahran, M. A.;
Ali, A. H.; El-Gaby, M. S. A.
CORPORATE SOURCE: Dep. Chemistry, Faculty Science, Al-Azhar Univ.,
Nasr-City, 11884, Egypt
SOURCE: Molecules [online computer file] (2001), 6(3), 267-278
CODEN: MOLEFW; ISSN: 1420-3049
URL: <http://www.mdpi.org/molecules/papers/60300267.pdf>
PUBLISHER: Molecular Diversity Preservation International
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
AB A number of novel triazino-, triazepino- and triazocinoquinazolinones were
obtained by nucleophilic reactions of 3-aminoquinazolinone derivs.
obtained by condensation of arylsulfonyl amino acids with Me anthranilate,
followed by hydrazinolysis. Some of the products showed antimicrobial and
antifungal activities.

RX(7) OF 76 ...C ==> P



C

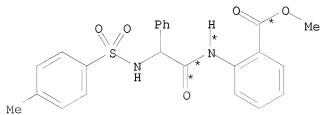
(7) \longrightarrow 

P

YIELD 74%

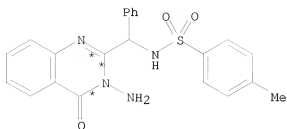
RX(7) RCT C 351333-19-2
 RGT Q 302-01-2 N2H4
 PRO P 276687-55-9
 SOL 7732-18-5 Water, 71-36-3 BuOH

RX(8) OF 76 ...G ==> T



G

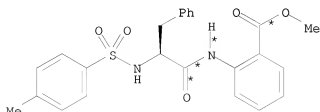
(8) \longrightarrow



T
YIELD 65%

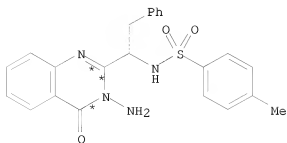
RX(8) RCT G 351333-20-5
 RGT Q 302-01-2 N2H4
 PRO T 351333-25-0
 SOL 7732-18-5 Water, 71-36-3 BuOH

RX(9) OF 76 ...I ==> U



I

(9) $\xrightarrow{\hspace{1cm}}$

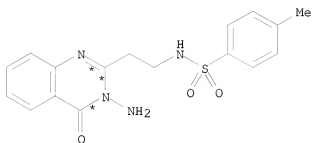
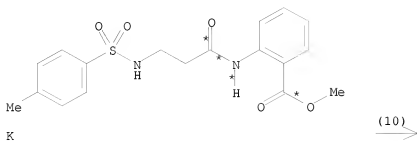


U
YIELD 68%

RX(9) RCT I 351333-21-6
 RGT Q 302-01-2 N2H4
 PRO U 351333-26-1
 SOL 7732-18-5 Water, 71-36-3 BuOH

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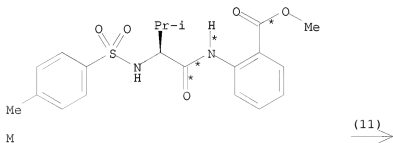
RX(10) OF 76 ...K ==> V...



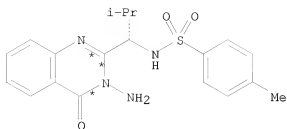
YIELD 70%

RX(10) RCT K 351333-22-7
 RGT Q 302-01-2 N2H4
 PRO V 351333-27-2
 SOL 7732-18-5 Water, 71-36-3 BuOH

RX(11) OF 76 ...M ==> W...



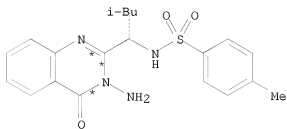
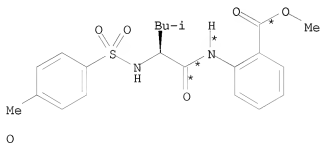
10/ 562,112



W
YIELD 76%

RX(11) RCT M 351333-23-8
 RGT Q 302-01-2 N2H4
 PRO W 351333-28-3
 SOL 7732-18-5 Water, 71-36-3 BuOH

RX(12) OF 76 ...O ==> X

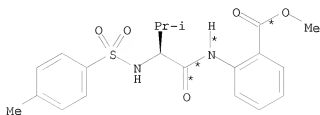


X
YIELD 71%

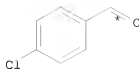
RX(12) RCT O 351333-24-9
 RGT Q 302-01-2 N2H4
 PRO X 351333-29-4
 SOL 7732-18-5 Water, 71-36-3 BuOH

10/ 562,112

RX(40) OF 76 COMPOSED OF RX(11), RX(21)
RX(40) M + AP ==> AQ

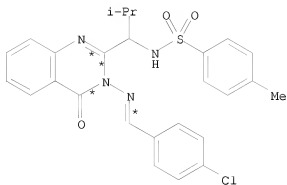


M



AP

2
STEPS
→



AQ
YIELD 69%

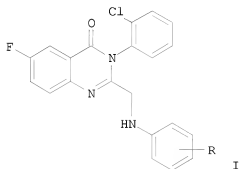
RX(11) RCT M 351333-23-8
RGT Q 302-01-2 N2H4
PRO W 351333-28-3
SOL 7732-18-5 Water, 71-36-3 BuOH

RX(21) RCT W 351333-28-3, AP 104-88-1
PRO AQ 351333-32-9
SOL 64-19-7 AcOH

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

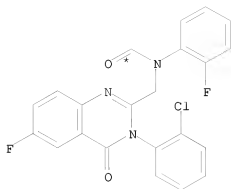
L3 ANSWER 106 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 135:76844 CASREACT
TITLE: Quinazolin-4-one

α -Amino-3-hydroxy-5-methyl-4-isoxazolepropionic
 Acid (AMPA) Receptor Antagonists: Structure-Activity
 Relationship of the C-2 Side Chain Tether
 AUTHOR(S): Chenard, Bertrand L.; Welch, Willard M.; Blake, James
 F.; Butler, Todd W.; Reinhold, Anthony; Ewing, Frank
 E.; Menniti, Frank S.; Pagnozzi, Martin J.
 CORPORATE SOURCE: Global Research and Development Groton Laboratories,
 Pfizer Inc., Groton, CT, 06340, USA
 SOURCE: Journal of Medicinal Chemistry (2001), 44(11),
 1710-1717
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



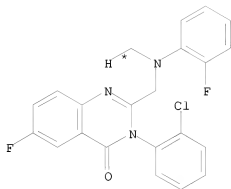
AB A series of 6-fluoro-3-(2-chlorophenyl)quinazolin-4-ones has been prepared, which contains a 2-fluorophenyl ring attached to C-2 by a variety of two-atom tethers. These compds. were used to probe the structure-activity relationship (SAR) for AMPA receptor inhibition. The relative potencies of the new compds. ranged from 11 nM to greater than 10 μ M. The differential activity of the compds. was rationalized on the basis of alterations of the 2-fluorophenyl positioning (planar and radial) relative to the quinazolin-4-one ring based on computational methods. From this effort, new AMPA receptor antagonists I [R = 2-F, 2-CN, 3-CN, 3-pyrrolidinomethyl], containing the methylamino tether group, have been identified.

RX(11) OF 53 ...AW ==> AX



AW

(11) \longrightarrow



AX

YIELD 30%

RX(11) RCT AW 346700-98-9

STAGE(1)

RGT AY 14044-65-6 BH3-THF

SOL 109-99-9 THF

CON 18 hours, room temperature

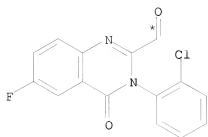
STAGE(2)

RGT AJ 67-56-1 MeOH

CON room temperature

PRO AX 346700-94-5

RX(16) OF 53 ...AD + BL ==> BM

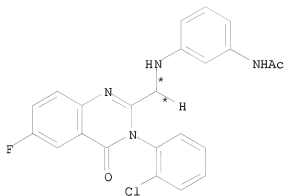


AD



BL

(16)

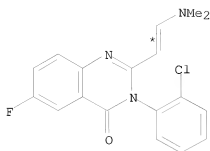


BM

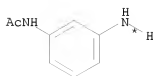
YIELD 29%

RX(16) RCT AD 217942-80-8, BL 102-28-3
 RGT AH 56553-60-7 Na.(AcO)3BH
 PRO BM 217942-64-8
 SOL 107-06-2 ClCH2CH2Cl
 CON 18 hours, room temperature

RX(33) OF 53 COMPOSED OF RX(17), RX(16)
 RX(33) BN + BL ==> BM

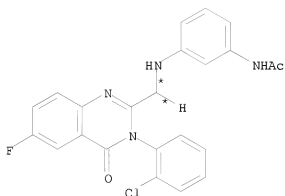


BN



BL

2
STEPS
→



BM

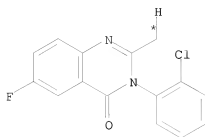
YIELD 29%

RX(17) RCT BN 217943-01-6
 RGT BO 7790-28-5 NaIO₄
 PRO AD 217942-80-8
 SOL 7732-18-5 Water, 109-99-9 THF
 CON SUBSTAGE(1) room temperature, pH 7
 SUBSTAGE(2) heated
 SUBSTAGE(3) 1 hour, room temperature
 NTE buffered solution, 1:2 mixture of free aldehyde and hydrate are formed

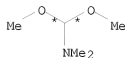
RX(16) RCT AD 217942-80-8, BL 102-28-3
 RGT AH 56553-60-7 Na.(AcO)₃BH
 PRO BM 217942-64-8
 SOL 107-06-2 ClCH₂CH₂Cl
 CON 18 hours, room temperature

RX(52) OF 53 COMPOSED OF RX(21), RX(17), RX(16)

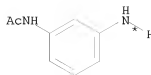
RX(52) A + BX + BL ==> BM



A

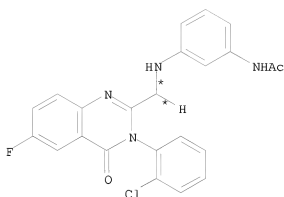


BX



BL

3
STEPS
→



BM

YIELD 29%

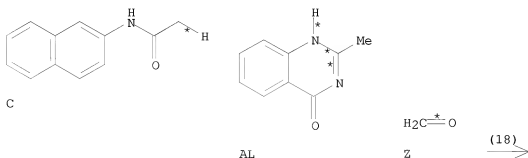
- RX(21) RCT A 49579-12-6, BX 4637-24-5
 PRO BN 217943-01-6
 SOL 68-12-2 DMF
 CON SUBSTAGE(1) 24 hours, 140 deg C
 SUBSTAGE(2) 140 deg C -> room temperature
 NTE thermal
- RX(17) RCT BN 217943-01-6
 RGT BO 7790-28-5 NaIO4
 PRO AD 217942-80-8
 SOL 7732-18-5 Water, 109-99-9 THF
 CON SUBSTAGE(1) room temperature, pH 7
 SUBSTAGE(2) heated
 SUBSTAGE(3) 1 hour, room temperature
 NTE buffered solution, 1:2 mixture of free aldehyde and hydrate are formed
- RX(16) RCT AD 217942-80-8, BL 102-28-3

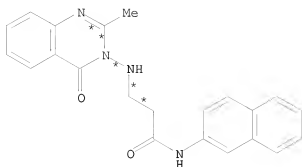
RGT AH 56553-60-7 Na.(AcO)3BH
 PRO BM 217942-64-8
 SOL 107-06-2 ClCH2CH2Cl
 CON 18 hours, room temperature

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 107 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 135:33439 CASREACT
 TITLE: Synthesis and anti-inflammatory activity of 1-acetyl-5-(substituted aryl)-3-(β -naphthylamino)-2-pyrazolines and [(substituted β -aminoethyl)amido]naphthalenes
 AUTHOR(S): Bansal, Ekta; Srivastava, V. K.; Kumar, Ashok
 CORPORATE SOURCE: Medicinal Chemistry Division, Department of Pharmacology, L.L.R.M. Medical College, Meerut, 250004, India
 SOURCE: European Journal of Medicinal Chemistry (2001), 36(1), 81-92
 CODEN: EJMCA5; ISSN: 0223-5234
 PUBLISHER: Editions Scientifiques et Medicales Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The title compds. were prepared by reaction of β -(acetylamino)naphthalene with aromatic aldehydes followed by cyclization with $N_2H_4 \cdot H_2O$ or by reaction with primary or secondary amines (Mannich reaction), resp. The structures of new compds. were confirmed by 1H -NMR and IR. Anti-inflammatory and ulcerogenic activities in vivo were evaluated and compared with the standard drugs phenylbutazone and indomethacin. Some compds. of the series exhibited promising anti-inflammatory activity with a lower ulcerogenic liability than the standard drugs.

RX(18) OF 66 ...C + AL + Z ==> AM



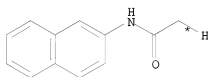


AM

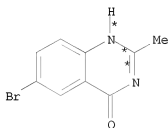
YIELD 40%

RX(18) RCT C 581-97-5, AL 1769-24-0, Z 50-00-0
 RGT T 302-01-2 N2H4
 PRO AM 343930-76-7
 SOL 64-17-5 EtOH

RX(19) OF 66 ...C + AN + Z ==> AO



C

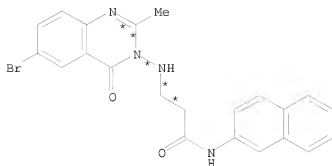


AN



Z

(19)



AO
YIELD 55%

RX(19) RCT C 581-97-5, AN 5426-59-5, Z 50-00-0
RGT T 302-01-2 N2H4
PRO AO 343930-77-8
SOL 64-17-5 EtOH

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 108 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 134:222305 CASREACT
TITLE: Stereoisomerism in

3-[N-(2-acetoxypropanoyl)-N-acylamino]quinazolin-4(3H)-ones, enantioselective acylating agents

AUTHOR(S): Al-Sehemi, Abdullah G.; Atkinson, Robert S.; Fawcett, John; Russell, David R.

CORPORATE SOURCE: Department of Chemistry, Leicester University, Leicester, LE1 7RH, UK

SOURCE: Perkin 1 (2000), (24), 4413-4421
CODEN: PERKF9; ISSN: 1470-4358

PUBLISHER: Royal Society of Chemistry

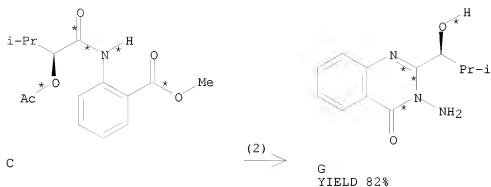
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The title compds. diacylaminoquinazolinones (DAQs) are enantioselective acylation agents for amines and a detailed study of their stereostructures was undertaken with the aim of understanding how this enantioselectivity arises. The N-N bond in these DAQs is a chiral axis. Even where both N-acyl groups are (S)-2-acetoxypropanoyl, the N-N bond is still a chiral axis because in the most stable conformation of the planar imide moiety, one exo/endo orientation of the carbonyl groups is much preferred over the alternative (endo/exo) as revealed by NMR spectroscopy. A conformational preference within the 2-acetoxypropanoyl grouping accounts for the presence of a single exo/endo conformation in solution for some of these DAQs (see above) but an interconverting exo/endo .dblharw. endo/exo mixture for others. Where a single exo/endo conformation is present in solution, evidence is presented that this closely resembles the X-ray determined crystal structure. A mechanism for the second acylation step to form these DAQs is proposed, which involves preliminary O-acylation of the 3-(monoacylamino)quinazolinone.

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RX(2) OF 18 ...C ==> G...



RX(2) RCT C 329729-34-2

STAGE(1)

RGT H 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

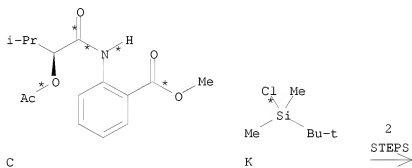
SOL 75-09-2 CH2Cl2

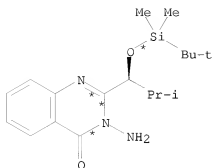
PRO G 329729-35-3

NTE stereoselective

RX(10) OF 18 COMPOSED OF RX(2), RX(3)

RX(10) C + K ==> L





L
YIELD 96%

RX(2) RCT C 329729-34-2

STAGE(1)

RGT H 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 75-09-2 CH2Cl2

PRO G 329729-35-3

NTE stereoselective

RX(3) RCT G 329729-35-3, K 18162-48-6

RGT M 288-32-4 1H-Imidazole

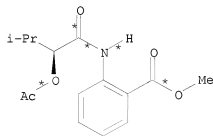
PRO L 262600-86-2

SOL 68-12-2 DMF

NTE stereoselective

RX(15) OF 18 COMPOSED OF RX(2), RX(3), RX(4)

RX(15) C + K + N ==> O



C

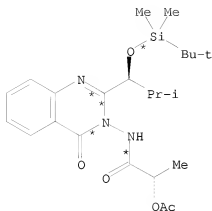


K



N

3
STEPS
→



O
YIELD 88%

RX(2) RCT C 329729-34-2

STAGE(1)

RGT H 302-01-2 N2H4
SOL 64-17-5 EtOH

STAGE(2)

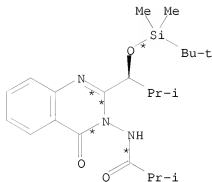
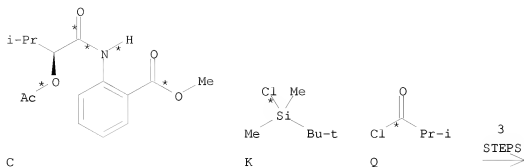
SOL 75-09-2 CH2Cl2

PRO G 329729-35-3
NTE stereoselective

RX(3) RCT G 329729-35-3, K 18162-48-6
RGT M 288-32-4 1H-Imidazole
PRO L 262600-86-2
SOL 68-12-2 DMF
NTE stereoselective

RX(4) RCT L 262600-86-2, N 36394-75-9
RGT P 110-86-1 Pyridine
PRO O 329729-36-4
SOL 75-09-2 CH2Cl2
NTE stereoselective

RX(16) OF 18 COMPOSED OF RX(2), RX(3), RX(5)
RX(16) C + K + Q ==> R



YIELD 79%

RX(2) RCT C 329729-34-2

STAGE(1)

RGT H 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 75-09-2 CH2Cl2

PRO G 329729-35-3

NTE stereoselective

RX(3) RCT G 329729-35-3, K 18162-48-6

RGT M 288-32-4 1H-Imidazole

PRO L 262600-86-2

SOL 68-12-2 DMF

NTE stereoselective

RX(5) RCT L 262600-86-2, Q 79-30-1

RGT P 110-86-1 Pyridine

PRO R 262600-88-4

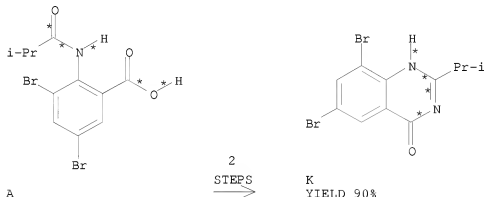
SOL 75-09-2 CH2Cl2

NTE stereoselective

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 109 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 134:157195 CASREACT
 TITLE: Synthesis and antifungal activity of some new quinazoline and benzoxazinone derivatives
 AUTHOR(S): Shalaby, Alyaa A.; El-Khamry, Abdel Momen A.; Shiba, S. A.; Ahmed, Abdel Aal Alm Eldeen Abdalah; Hanafi, Awaref A.
 CORPORATE SOURCE: Chemistry Department, Faculty of Science, Ain Shams University, Cairo, Egypt
 SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2000), 333(11), 365-372
 CODEN: ARPMAS; ISSN: 0365-6233
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The hitherto unknown 2-isopropyl-6,8-dibromo-4H-3,1-benzoxazin-4-one was subjected to condensation with either primary or secondary amines affording the benzamide derivs., while with alcs. in presence of the base, corresponding esters were obtained. A series of other compds. were also prepared according to the methods discussed in the text. Ten of our compds. were examined against *Sclerotium cepivorum* as well as *Botrytis allii* on PDA media. These compds. showed a significant reduction of mycelial growth and sclerotia number of these fungi which cause the white rot and neck rot diseases of onion.

RX(34) OF 113 COMPOSED OF RX(1), RX(5)
 RX(34) A ==> K



RX(1) RCT A 325707-07-1
 PRO B 325707-08-2
 SOL 108-24-7 Ac2O
 NTE PETROLEUM USED

RX(5) RCT B 325707-08-2

STAGE(1)

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RGT L 631-61-8 NH4OAc

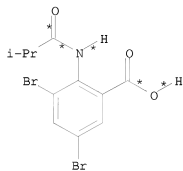
STAGE(2)

SOL 7732-18-5 Water

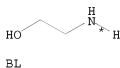
PRO K 325707-24-2

RX(39) OF 113 COMPOSED OF RX(1), RX(28)

RX(39) A + BL ==> N

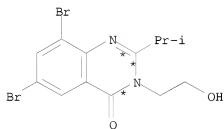


A



BL

2
STEPS
→



N

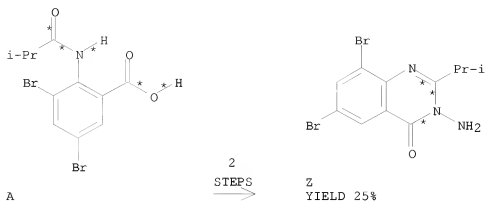
YIELD 60%

RX(1) RCT A 325707-07-1
PRO B 325707-08-2
SOL 108-24-7 Ac2O
NTE PETROLEUM USED

RX(28) RCT B 325707-08-2, BL 141-43-5
PRO N 325707-16-2
NTE PETROLEUM USED

RX(40) OF 113 COMPOSED OF RX(1), RX(29)

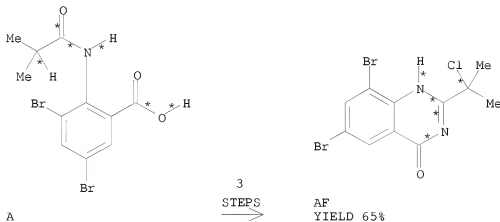
RX(40) A ==> Z



RX(1) RCT A 325707-07-1
 PRO B 325707-08-2
 SOL 108-24-7 Ac2O
 NTE PETROLEUM USED

RX(29) RCT B 325707-08-2
 RGT BM 7803-57-8 N2H4-H2O
 PRO Z 325707-19-5
 SOL 64-17-5 EtOH

RX(59) OF 113 COMPOSED OF RX(1), RX(5), RX(13)
 RX(59) A ==> AF



RX(1) RCT A 325707-07-1
 PRO B 325707-08-2
 SOL 108-24-7 Ac2O
 NTE PETROLEUM USED

RX(5) RCT B 325707-08-2

STAGE(1)
 RGT L 631-61-8 NH4OAc

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STAGE(2)

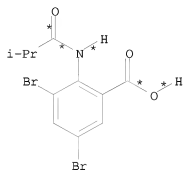
SOL 7732-18-5 Water

PRO K 325707-24-2

RX(13) RCT K 325707-24-2
RGT AG 10025-87-3 POC13, AH 10026-13-8 PC15
PRO AF 325707-36-6
SOL 108-88-3 PhMe

RX(60) OF 113 COMPOSED OF RX(1), RX(28), RX(6)

RX(60) A + BL ==> O

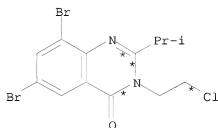


A



BL

3
STEPS
→



O

YIELD 70%

RX(1) RCT A 325707-07-1
PRO B 325707-08-2
SOL 108-24-7 Ac2O
NTE PETROLEUM USED

RX(28) RCT B 325707-08-2, BL 141-43-5
PRO N 325707-16-2
NTE PETROLEUM USED

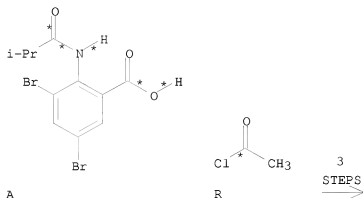
RX(6) RCT N 325707-16-2
RGT P 7719-09-7 SOC12

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PRO O 325707-17-3

RX(61) OF 113 COMPOSED OF RX(1), RX(29), RX(10)

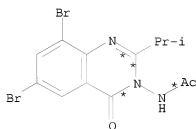
RX(61) A + R ==> AA



A

R

3
STEPS
→



AA

YIELD 65%

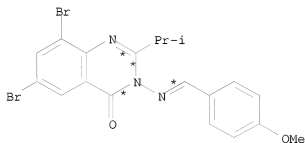
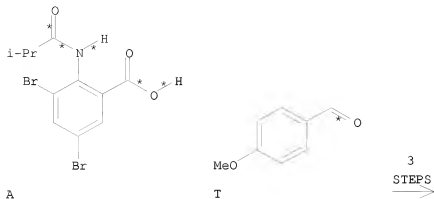
RX(1) RCT A 325707-07-1
PRO B 325707-08-2
SOL 108-24-7 Ac2O
NTE PETROLEUM USED

RX(29) RCT B 325707-08-2
RGT BM 7803-57-8 N2H4-H2O
PRO Z 325707-19-5
SOL 64-17-5 EtOH

RX(10) RCT Z 325707-19-5, R 75-36-5
PRO AA 325707-21-9

RX(62) OF 113 COMPOSED OF RX(1), RX(29), RX(11)

RX(62) A + T ==> AB



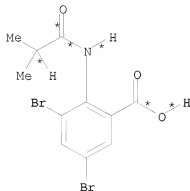
YIELD 75%

RX(1) RCT A 325707-07-1
 PRO B 325707-08-2
 SOL 108-24-7 Ac2O
 NTE PETROLEUM USED

RX(29) RCT B 325707-08-2
 RGT BM 7803-57-8 N2H4-H2O
 PRO Z 325707-19-5
 SOL 64-17-5 EtOH

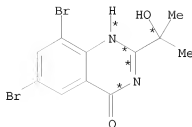
RX(11) RCT Z 325707-19-5, T 123-11-5
 PRO AB 325707-23-1
 SOL 64-17-5 EtOH

RX(85) OF 113 COMPOSED OF RX(1), RX(5), RX(13), RX(22)
 RX(85) A ==> AY



A

4
STEPS
→



AY
YIELD 80%

RX(1) RCT A 325707-07-1
PRO B 325707-08-2
SOL 108-24-7 Ac2O
NTE PETROLEUM USED

RX(5) RCT B 325707-08-2

STAGE(1)
RGT L 631-61-8 NH4OAc

STAGE(2)
SOL 7732-18-5 Water

PRO K 325707-24-2

RX(13) RCT K 325707-24-2
RGT AG 10025-87-3 POC13, AH 10026-13-8 PC15
PRO AF 325707-36-6
SOL 108-88-3 PhMe

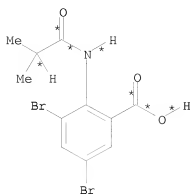
RX(22) RCT AF 325707-36-6

STAGE(1)
RGT AL 497-19-8 Na2CO3
SOL 7732-18-5 Water

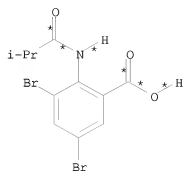
STAGE(2)
RGT AZ 7697-37-2 HNO3

PRO AY 325707-37-7

RX(100) OF 113 COMPOSED OF RX(1), RX(5), RX(12), RX(19), RX(20)
RX(100) 2 A ==> AF

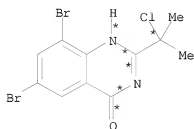


A



A

5
STEPS
→



AF
YIELD 80%

RX(1) RCT A 325707-07-1
PRO B 325707-08-2
SOL 108-24-7 Ac2O
NTE PETROLEUM USED

RX(5) RCT B 325707-08-2

STAGE(1)
RGT L 631-61-8 NH4OAc

STAGE(2)
SOL 7732-18-5 Water

PRO K 325707-24-2

RX(12) RCT K 325707-24-2
RGT AD 19172-47-5 Lawesson's reagent
PRO AC 325707-26-4
SOL 108-88-3 PhMe

RX(19) RCT AC 325707-26-4
RGT AG 10025-87-3 POC13, AH 10026-13-8 PC15
PRO AU 325707-34-4, AV 325707-35-5

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RX(20) RCT AV 325707-35-5

STAGE(1)

RGT AW 26628-22-8 NaN3

SOL 64-19-7 AcOH

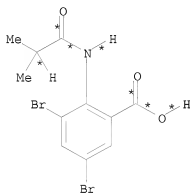
STAGE(2)

SOL 7732-18-5 Water

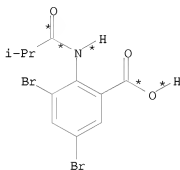
PRO AF 325707-36-6

RX(112) OF 113 COMPOSED OF RX(1), RX(5), RX(12), RX(19), RX(20), RX(22)

RX(112) 2 A ==> AY

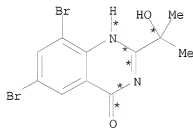


A



A

6
STEPS
→



AY

YIELD 80%

RX(1) RCT A 325707-07-1
PRO B 325707-08-2
SOL 108-24-7 Ac2O
NTE PETROLEUM USED

RX(5) RCT B 325707-08-2

STAGE(1)

RGT L 631-61-8 NH4OAc

STAGE(2)
 SOL 7732-18-5 Water

PRO K 325707-24-2

RX(12) RCT K 325707-24-2
 RGT AD 19172-47-5 Lawesson's reagent
 PRO AC 325707-26-4
 SOL 108-88-3 PhMe

RX(19) RCT AC 325707-26-4
 RGT AG 10025-87-3 POC13, AH 10026-13-8 PC15
 PRO AU 325707-34-4, AV 325707-35-5

RX(20) RCT AV 325707-35-5

STAGE(1)
 RGT AW 26628-22-8 NaN3
 SOL 64-19-7 AcOH

STAGE(2)
 SOL 7732-18-5 Water

PRO AF 325707-36-6

RX(22) RCT AF 325707-36-6

STAGE(1)
 RGT AL 497-19-8 Na2CO3
 SOL 7732-18-5 Water

STAGE(2)
 RGT AZ 7697-37-2 HNO3

PRO AY 325707-37-7

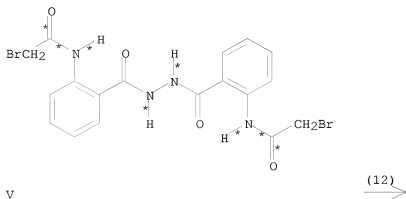
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 110 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 134:100515 CASREACT
 TITLE: Tetraacyl hydrazines and
 3,3'-biquinazoline-4,4'-diones; synthesis, studies of
 rotational barriers and deracemisation
 AUTHOR(S): Coogan, Michael P.; Passey, Steven C.
 CORPORATE SOURCE: Science Laboratories, Department of Chemistry,
 University of Durham, Durham, DH1 3LE, UK
 SOURCE: Perkin 2 (2000), (10), 2060-2066
 CODEN: PRKTFQ; ISSN: 1470-1820
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The barrier to rotation around the N-N bond in
 3,3'-biquinazoline-4,4'-dione is estimated to be 96 kJ mol⁻¹, significantly
 higher than in acyclic tetraacyl hydrazines (84 kJ mol⁻¹). Both dynamic
 chiroptical and NMR studies of 3,3'-biquinazoline-4,4'-diones which have

an addnl. ring bridging the 2,2' positions indicate that these compds. have a significantly higher barrier to rotation than the parent 3,3'-biquinazoline-4,4'-dione. Deracemization of certain 3,3'-biquinazoline-4,4'-diones is possible via treatment with chiral acids at high temperature

RX(12) OF 34 ...V ==> AE...



AE
YIELD 81%

RX(12) RCT V 319426-05-6

STAGE(1)
RGT AM 104-15-4 TsOH
SOL 108-88-3 PhMe

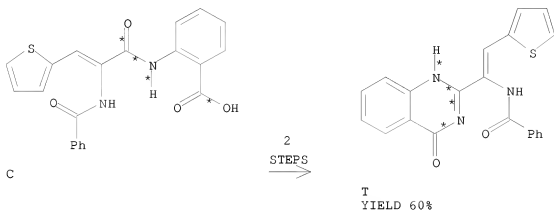
STAGE(2)
SOL 141-78-6 AcOEt

PRO AE 253141-07-0

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 134:86206 CASREACT
 TITLE: The behaviour of some nucleophiles towards
 2-[α -(benzoylamino)- β -(2-thienyl)vinyl]benzoxazin-4(3H)-one
 AUTHOR(S): Guirguis, Dalal B.
 CORPORATE SOURCE: Chemistry Department, Faculty of Science, Ain Shams
 University, Cairo, Egypt
 SOURCE: Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (2000),
 39B(4), 264-269
 CODEN: IJSBDB; ISSN: 0376-4699
 PUBLISHER: National Institute of Science Communication, CSIR
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 2-[α -(Benzoylamino)- β -thien-2-ylvinyl]benzoxazin-4(3H)-one (I)
 undergoes ring-opening on treatment with primary and secondary amines
 affording 2-[α -(benzoylamino)- β -thien-2-ylacrylamido]benzamides. Treatment of I with HCONH₂ and N₂H₄·H₂O at
 elevated temperature gives rise to quinazolinones. Interestingly, reaction of
 vicinal aminobenzyl alcs. with I yields the usual ring-opening products
 and unexpected 4-iminobenzoxazines.

RX(29) OF 80 COMPOSED OF RX(2), RX(9)
 RX(29) C ==> T



RX(2) RCT C 318292-63-6

STAGE(1)
 SOL 108-24-7 Ac₂O

STAGE(2)
 SOL 7732-18-5 Water

PRO F 318292-64-7

RX(9) RCT F 318292-64-7

STAGE(1)
 RGT U 75-12-7 Formamide
 SOL 64-17-5 EtOH

10/ 562,112

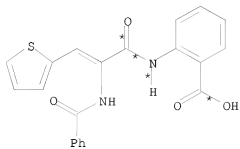
STAGE(2)

SOL 7732-18-5 Water

PRO T 318292-72-7

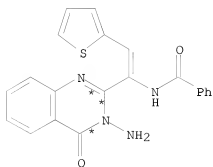
RX(30) OF 80 COMPOSED OF RX(2), RX(10)

RX(30) C ==> V



C

2
STEPS
→



V

YIELD 60%

RX(2) RCT C 318292-63-6

STAGE(1)

SOL 108-24-7 Ac2O

STAGE(2)

SOL 7732-18-5 Water

PRO F 318292-64-7

RX(10) RCT F 318292-64-7

RGT I 302-01-2 N2H4

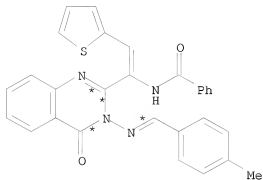
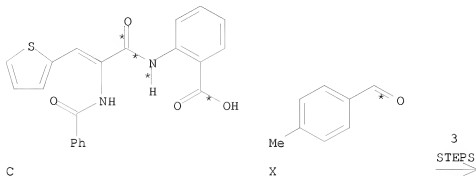
PRO V 318292-73-8

SOL 71-36-3 BuOH

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RX(74) OF 80 COMPOSED OF RX(2), RX(10), RX(11)

RX(74) C + X ==> Y



YIELD 40%

RX(2) RCT C 318292-63-6

STAGE(1)

SOL 108-24-7 Ac2O

STAGE(2)

SOL 7732-18-5 Water

PRO F 318292-64-7

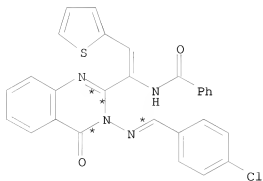
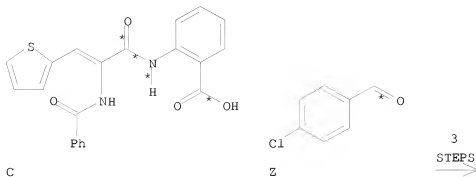
RX(10) RCT F 318292-64-7
RGT I 302-01-2 N2H4
PRO V 318292-73-8
SOL 71-36-3 BuOH

RX(11) RCT V 318292-73-8, X 104-87-0
PRO Y 318292-74-9
CAT 110-89-4 Piperidine
SOL 64-17-5 EtOH

RX(75) OF 80 COMPOSED OF RX(2), RX(10), RX(12)

10/ 562,112

RX(75) C + Z ==> AA



AA
YIELD 48%

RX(2) RCT C 318292-63-6

STAGE(1)
SOL 108-24-7 Ac2O

STAGE(2)
SOL 7732-18-5 Water

PRO F 318292-64-7

RX(10) RCT F 318292-64-7
RGT I 302-01-2 N2H4
PRO V 318292-73-8
SOL 71-36-3 BuOH

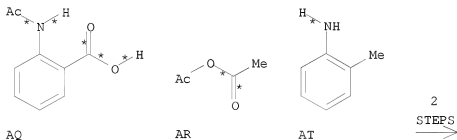
RX(12) RCT V 318292-73-8, Z 104-88-1
PRO AA 318292-75-0
CAT 110-89-4 Piperidine
SOL 64-17-5 EtOH

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 112 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 134:72897 CASREACT
 TITLE: Synthesis of 2-methyl-3-(2'-methylphenyl)-6-aryl
 azo-4-oxoquinazoline derivatives and their application
 AUTHOR(S): Patel, R. B.; Patel, Nilesh; Patel, S. K.; Patel, K.
 C.
 CORPORATE SOURCE: Department of Chemistry, South Gujarat University,
 Surat, 395 007, India
 SOURCE: Oriental Journal of Chemistry (2000), 16(2), 305-310
 CODEN: OJCHEG; ISSN: 0970-020X
 PUBLISHER: Oriental Scientific Publishing Co.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A series of dyes has been prepared by coupling of diazotized
 2-methyl-3-(2-methylphenyl)-6-amino-4-oxoquinazoline with various coupling
 components to give 4-oxoquinazoline-based azo dyes and their dyeing
 performance on silk, wool, and rayon has been assessed. These dyes have
 been found to give a variety of color shades with very good depth and
 levelness on the fibers. The IR spectra showed all characteristic bands
 and a representative dye PMR spectrum showed all the expected signals.
 The percentage dye-bath exhaustion and fixation on different fibers was
 reasonably good and acceptable, resp. The dyed fibers showed good to
 excellent fastness to light, washing, and rubbing.

RX(22) OF 95 COMPOSED OF RX(18), RX(19)

RX(22) AQ + AR + AT ==> AU



AU
 YIELD 89%

RX(18) RCT AQ 89-52-1, AR 108-24-7
 PRO AS 525-76-8

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RX(19) RCT AS 525-76-8, AT 95-53-4

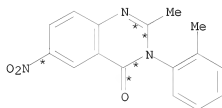
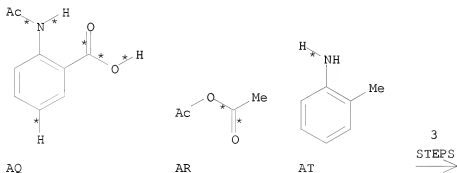
STAGE (1)

STAGE (2)

RGT D 7647-01-0 HCL

PRO AU 72-44-6

RX(42) OF 95 COMPOSED OF RX(18), RX(19), RX(20)

$$RX(42) \quad AQ + AR + AT \implies AV$$


AV
YIELD 95%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE (1)

STAGE (2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE (1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

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STAGE(2)

SOL 7732-18-5 Water

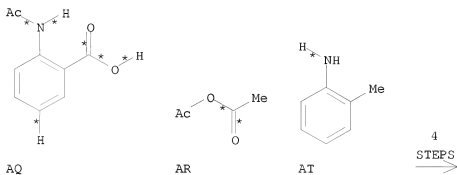
STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(44) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21)

RX(44) AQ + AR + AT ==> A



A
YIELD 88%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

10/ 562,112

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

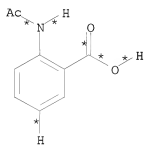
RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

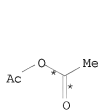
PRO A 963-34-8

RX(79) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(1)

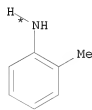
RX(79) AQ + AR + AT + B ==> C



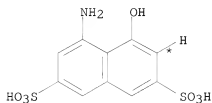
AQ



AR

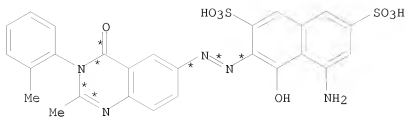


AT



B

5
STEPS
→



● 2 Na

C

YIELD 86%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(1) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

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SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT B 90-20-0

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

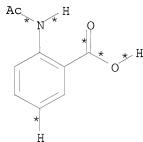
RGT H 7647-14-5 NaCl

STAGE(7)

SOL 68-12-2 DMF

PRO C 313697-89-1

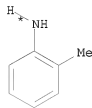
RX(80) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(2)
RX(80) AQ + AR + AT + K ==> L



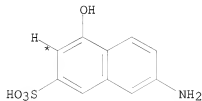
AQ



AR

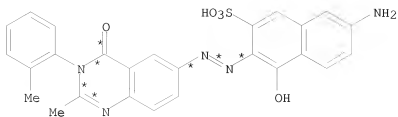


AT



K

5
STEPS
→



● Na

L

YIELD 79%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(2) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

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SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT K 87-02-5

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

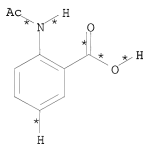
RGT H 7647-14-5 NaCl

STAGE(7)

SOL 68-12-2 DMF

PRO L 313697-90-4

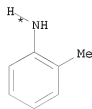
RX(81) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(3)
 RX(81) AQ + AR + AT + M ==> N



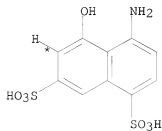
AQ



AR

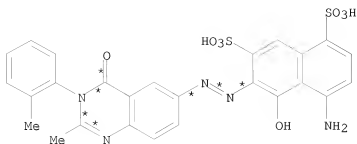


AT



M

5
STEPS
→



● 2 Na

N

YIELD 75%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(3) RCT A 963-34-8

STAGE(1)

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RGT D 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)
RGT E 7632-00-0 NaNO2
SOL 7732-18-5 Water

STAGE(3)
RGT F 5329-14-6 Sulfamic acid

STAGE(4)
RCT M 130-23-4
SOL 7732-18-5 Water

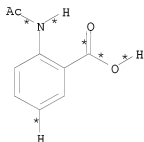
STAGE(5)
RGT G 497-19-8 Na2CO3

STAGE(6)
RGT H 7647-14-5 NaCl

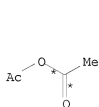
STAGE(7)
SOL 68-12-2 DMF

PRO N 313697-91-5

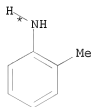
RX(82) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(4)
RX(82) AQ + AR + AT + O ==> P



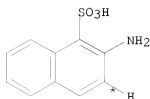
AQ



AR

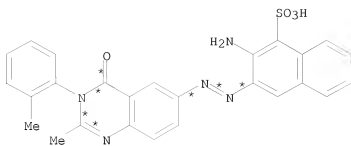


AT



O

5
STEPS
=>



P
YIELD 82%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(4) RCT A 963-34-8

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STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO₂

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT O 81-16-3

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na₂CO₃

STAGE(6)

RGT H 7647-14-5 NaCl

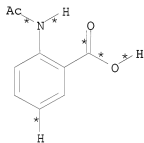
STAGE(7)

SOL 68-12-2 DMF

PRO P 313697-92-6

RX(83) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(5)

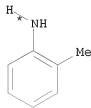
RX(83) AQ + AR + AT + Q ==> R



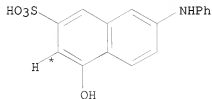
AQ



AR

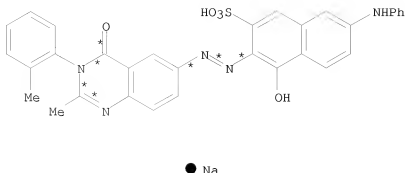


AT



Q

5
STEPS
➞



R

YIELD 84%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H₂SO₄, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na₂S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(5) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

10/ 562,112

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT Q 119-40-4

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

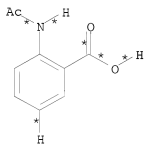
STAGE(7)

SOL 68-12-2 DMF

PRO R 313697-93-7

RX(84) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(6)

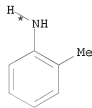
RX(84) AQ + AR + AT + S ==> T



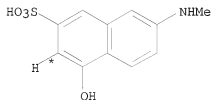
AQ



AR

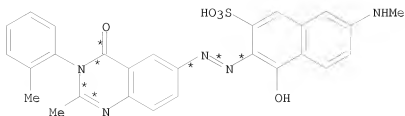


AT



S

5
STEPS
→



● Na

T

YIELD 76%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(6) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

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SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT S 22346-43-6

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

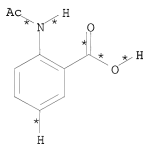
RGT H 7647-14-5 NaCl

STAGE(7)

SOL 68-12-2 DMF

PRO T 313697-94-8

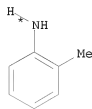
RX(85) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(7)
RX(85) AQ + AR + AT + U ==> V



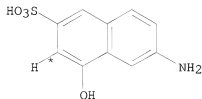
AQ



AR

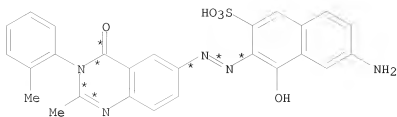


AT



U

5
STEPS
→



● Na

V

YIELD 87%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(7) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

10/ 562,112

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT U 90-51-7

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

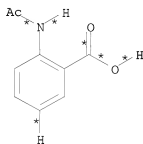
STAGE(7)

SOL 68-12-2 DMF

PRO V 313697-95-9

RX(86) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(8)

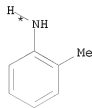
RX(86) AQ + AR + AT + W ==> X



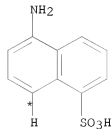
AQ



AR

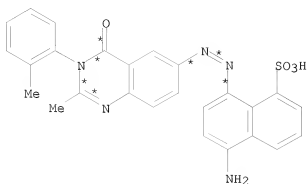


AT



W

5
STEPS
→



X
YIELD 78%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(8) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT W 84-89-9

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

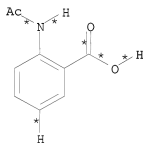
STAGE(7)

SOL 68-12-2 DMF

PRO X 313697-96-0

RX(87) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(9)

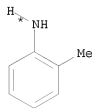
RX(87) AQ + AR + AT + Y ==> Z



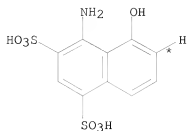
AQ



AR

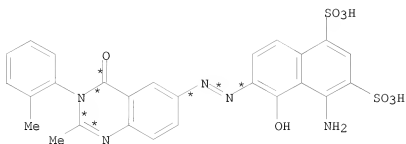


AT



Y

5
STEPS
→



● 2 Na

Z

YIELD 88%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(9) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT Y 82-47-3

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

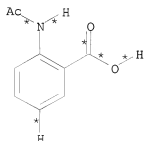
STAGE(7)

SOL 68-12-2 DMF

PRO Z 313697-97-1

RX(88) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(10)

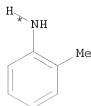
RX(88) AQ + AR + AT + AA ==> AB



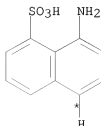
AQ



AR



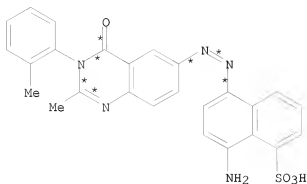
AT



AA

10/ 562,112

5
STEPS
→



● Na

AB
YIELD 77%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H₂SO₄, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na₂S

SOL 7732-18-5 Water

10/ 562,112

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(10) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AA 82-75-7

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

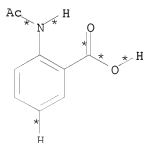
STAGE(7)

SOL 68-12-2 DMF

PRO AB 313697-98-2

RX(89) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(11)

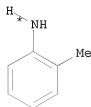
RX(89) AQ + AR + AT + AC ==> AD



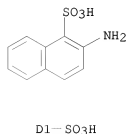
AQ



AR

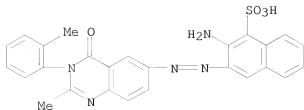


AT



AC

5
STEPS
→

D1- SO₃H

● 2 Na

AD

YIELD 72%

RX(18) RCT AQ 89-52-1, AR 108-24-7
 PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H₂SO₄, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na₂S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(11) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2
SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AC 171570-11-9
SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

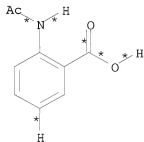
RGT H 7647-14-5 NaCl

STAGE(7)

SOL 68-12-2 DMF

PRO AD 314730-80-8

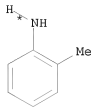
RX(90) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(12)
RX(90) AQ + AR + AT + AE ==> AF



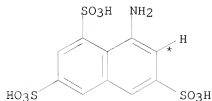
AQ



AR

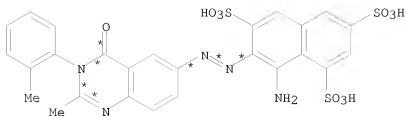


AT



AE

5
STEPS
→



● 3 Na

AF

YIELD 78%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(12) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

10/ 562,112

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AE 117-42-0

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

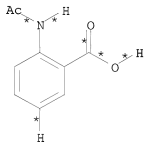
RGT H 7647-14-5 NaCl

STAGE(7)

SOL 68-12-2 DMF

PRO AF 313697-99-3

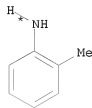
RX(91) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(13)
RX(91) AQ + AR + AT + AG ==> AH



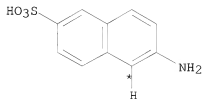
AQ



AR

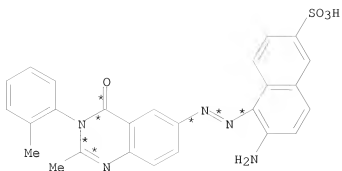


AT



AG

5
STEPS
=>



● Na

AH

YIELD 83%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H₂SO₄, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na₂S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

10/ 562,112

RX(13) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AG 93-00-5

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

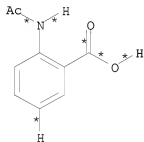
STAGE(7)

SOL 68-12-2 DMF

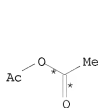
PRO AH 313698-00-9

RX(92) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(14)

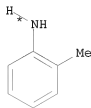
RX(92) AQ + AR + AT + AI ==> AJ



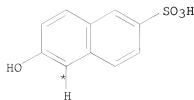
AQ



AR

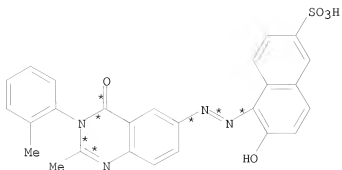


AT



AI

5
STEPS
→



AJ

YIELD 86%

RX(18) RCT AQ 89-52-1, AR 108-24-7
 PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

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RX(14) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AI 93-01-6

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

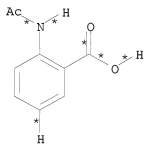
STAGE(7)

SOL 68-12-2 DMF

PRO AJ 313698-01-0

RX(93) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(15)

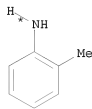
RX(93) AQ + AR + AT + AK ==> AL



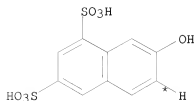
AQ



AR

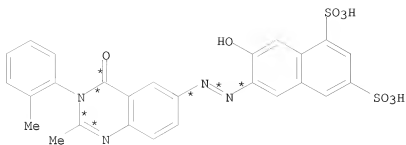


AT



AK

5
STEPS
=>



● 2 Na

AL
YIELD 82%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

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RX(15) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AK 118-32-1

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

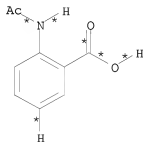
STAGE(7)

SOL 68-12-2 DMF

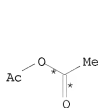
PRO AL 313698-02-1

RX(94) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(16)

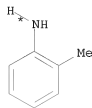
RX(94) AQ + AR + AT + AM ==> AN



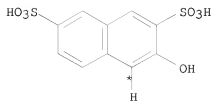
AQ



AR

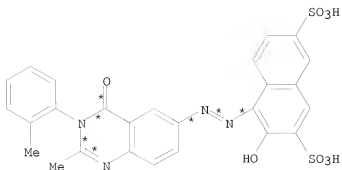


AT



AM

5
STEPS
→



● 2 Na

AN

YIELD 75%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

10/ 562,112

RX(16) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2

SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AM 148-75-4

SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

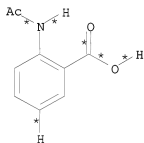
STAGE(7)

SOL 68-12-2 DMF

PRO AN 313698-03-2

RX(95) OF 95 COMPOSED OF RX(18), RX(19), RX(20), RX(21), RX(17)

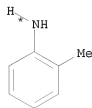
RX(95) AQ + AR + AT + AO ==> AP



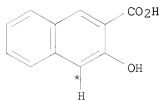
AQ



AR

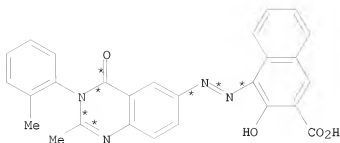


AT



AO

5
STEPS
→



● Na

AP
YIELD 81%

RX(18) RCT AQ 89-52-1, AR 108-24-7
PRO AS 525-76-8

RX(19) RCT AS 525-76-8, AT 95-53-4

STAGE(1)

STAGE(2)

RGT D 7647-01-0 HCl

PRO AU 72-44-6

RX(20) RCT AU 72-44-6

STAGE(1)

RGT AW 7664-93-9 H2SO4, J 68-12-2 DMF

STAGE(2)

SOL 7732-18-5 Water

STAGE(3)

RGT AX 64-19-7 AcOH

PRO AV 1038-69-3

RX(21) RCT AV 1038-69-3

STAGE(1)

RGT AY 1313-82-2 Na2S

SOL 7732-18-5 Water

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water

PRO A 963-34-8

RX(17) RCT A 963-34-8

STAGE(1)

RGT D 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)

RGT E 7632-00-0 NaNO2
SOL 7732-18-5 Water

STAGE(3)

RGT F 5329-14-6 Sulfamic acid

STAGE(4)

RCT AO 92-70-6
SOL 7732-18-5 Water

STAGE(5)

RGT G 497-19-8 Na2CO3

STAGE(6)

RGT H 7647-14-5 NaCl

STAGE(7)

SOL 68-12-2 DMF

PRO AP 313698-04-3

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 113 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 134:72894 CASREACT

TITLE: Quinazoline dyes: synthesis of
2-styryl-6-arylaazo-4-oxoquinazoline dyes and their
application on silk, wool and viscose rayonAUTHOR(S): Patel, K. C.; Patel, S. K.; Desai, K. R.
CORPORATE SOURCE: Department of Chemistry, South Gujarat University,
Surat, 395007, IndiaSOURCE: Acta Ciencia Indica, Chemistry (1999), 25(3), 41-48
CODEN: ACICDV; ISSN: 0253-7338

PUBLISHER: Pragati Prakashan

DOCUMENT TYPE: Journal

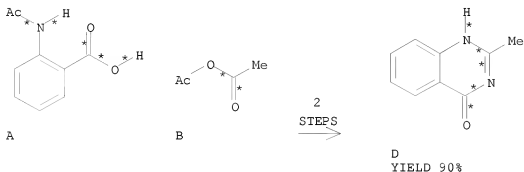
LANGUAGE: English

AB Various quinazoline dyes have been prepared by coupling of diazotized 2-styryl-6-amino-4-oxoquinazoline with various coupling components such as H-acid, J-acid, N-methyl-J-acid, N-phenyl-J-acid, Gamma acid, G-acid, R-salt, Schaffer's acid, 1-phenyl-3-methyl-5-pyrazolone, 1-(4'-sulfophenyl)-3-methyl-5-pyrazolone, 1-(2',5'-dichloro-4'-sulfophenyl)-3-methyl-5-pyrazolone, 1-(4'-sulfophenyl)-3-carboxy-5-pyrazolone and peri acid and their dyeing performance of direct dyes has been assessed on viscose rayon and as acid dyes has been assessed on silk and wool fibers. The purity of all dyes have been checked by thin-layer chromatog. The value of percentage found of N of all these dyes is in good agreement with the calculated values. The IR spectra of all these dyes showed all characteristic band present in the dye mols. The % exhaustion of dye-bath on silk and wool was good to

excellent and on viscose rayon it was poor to moderate. A study of the fastness of dyed patterns showed that the dyes were good to very good for silk and wool, and fair to good for viscose rayon.

RX(19) OF 93 COMPOSED OF RX(1), RX(2)

RX(19) A + B ==> D



RX(1) RCT A 89-52-1, B 108-24-7

PRO C 525-76-8

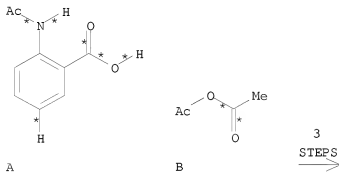
RX(2) RCT C 525-76-8

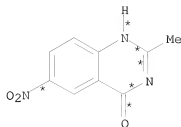
RGT E 7664-41-7 NH3

PRO D 1769-24-0

RX(36) OF 93 COMPOSED OF RX(1), RX(2), RX(3)

RX(36) A + B ==> F





F
YIELD 95%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

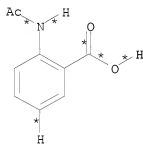
RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(38) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4)
RX(38) A + B + J ==> K



A

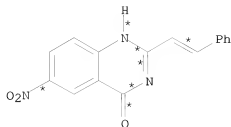


B



J

4
STEPS
→



K
YIELD 80%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

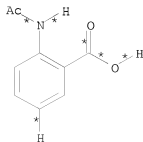
RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(67) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5)
RX(67) A + B + J ==> L



A

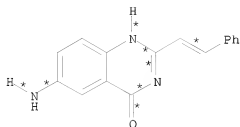


B



J

5
STEPS
→



L
YIELD 88%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

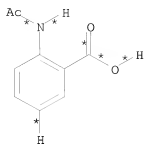
STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3
RGT M 1313-82-2 Na2S
PRO L 30896-48-1
SOL 7732-18-5 Water

RX(81) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6)
RX(81) A + B + J + N ==> O



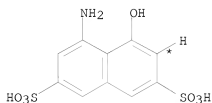
A



B

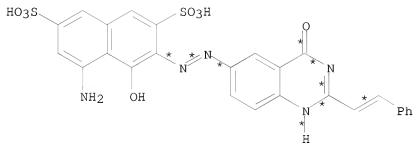


J



N

6
STEPS
→



O

YIELD 84%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)
RGT B 108-24-7 Ac2O

STAGE(2)
RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3
RGT M 1313-82-2 Na2S
PRO L 30896-48-1
SOL 7732-18-5 Water

RX(6) RCT L 30896-48-1

STAGE(1)
RGT P 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)
RGT Q 7632-00-0 NaNO2

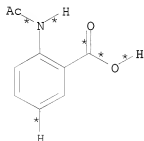
STAGE(3)
RGT G 7664-93-9 H2SO4

STAGE(4)
RCT N 90-20-0
RGT R 144-55-8 NaHCO3
SOL 7732-18-5 Water

STAGE(5)
RGT S 7647-14-5 NaCl

PRO O 315681-02-8

RX(82) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(7)
RX(82) A + B + J + T ==> U



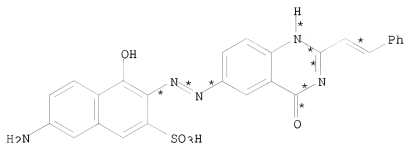
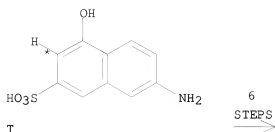
A



B



J



U
YIELD 81%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)
RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)
SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)
RGT B 108-24-7 Ac2O

STAGE(2)
RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3
RGT M 1313-82-2 Na2S
PRO L 30896-48-1
SOL 7732-18-5 Water

10/ 562,112

RX(7) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT Q 7632-00-0 NaNO2

STAGE(3)

RGT G 7664-93-9 H2SO4

STAGE(4)

RCT T 87-02-5

RGT R 144-55-8 NaHCO3

SOL 7732-18-5 Water

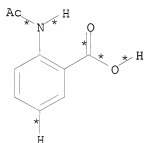
STAGE(5)

RGT S 7647-14-5 NaCl

PRO U 315681-03-9

RX(83) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(8)

RX(83) A + B + J + V ==> W



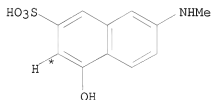
A



B

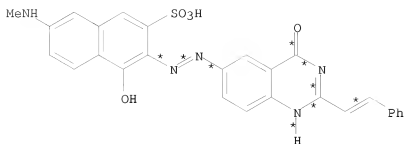


J



V

6
STEPS
→



W

YIELD 82%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3
RGT M 1313-82-2 Na2S
PRO L 30896-48-1
SOL 7732-18-5 Water

RX(8) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT Q 7632-00-0 NaNO2

STAGE(3)

RGT G 7664-93-9 H2SO4

10/ 562,112

STAGE(4)

RCT V 22346-43-6

RGT R 144-55-8 NaHCO₃

SOL 7732-18-5 Water

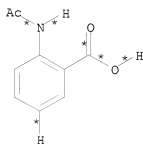
STAGE(5)

RGT S 7647-14-5 NaCl

PRO W 315681-04-0

RX(84) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(9)

RX(84) A + B + J + X ==> Y



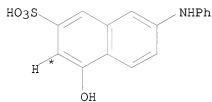
A



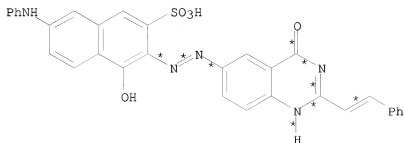
B



J



X



Y

YIELD 86%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3
RGT M 1313-82-2 Na2S
PRO L 30896-48-1
SOL 7732-18-5 Water

RX(9) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT Q 7632-00-0 NaNO2

STAGE(3)

RGT G 7664-93-9 H2SO4

STAGE(4)

RCT X 119-40-4

RGT R 144-55-8 NaHCO3

SOL 7732-18-5 Water

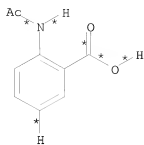
STAGE(5)

RGT S 7647-14-5 NaCl

PRO Y 315681-05-1

RX(85) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(10)

RX(85) A + B + J + Z ==> AA



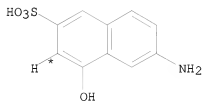
A



B

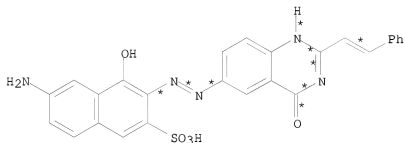


J



Z

6
STEPS
→



AA

YIELD 81%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)
RGT B 108-24-7 Ac2O

STAGE(2)
RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3
RGT M 1313-82-2 Na2S
PRO L 30896-48-1
SOL 7732-18-5 Water

RX(10) RCT L 30896-48-1

STAGE(1)
RGT P 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)
RGT Q 7632-00-0 NaNO2

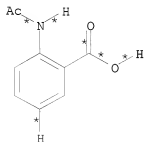
STAGE(3)
RGT G 7664-93-9 H2SO4

STAGE(4)
RCT Z 90-51-7
RGT R 144-55-8 NaHCO3
SOL 7732-18-5 Water

STAGE(5)
RGT S 7647-14-5 NaCl

PRO AA 315681-06-2

RX(86) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(11)
RX(86) A + B + J + AB ==> AC



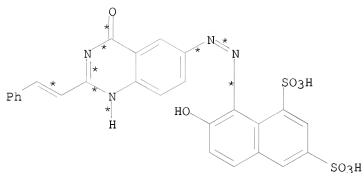
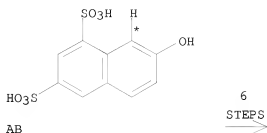
A



B



J



RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3
RGT M 1313-82-2 Na2S

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PRO L 30896-48-1
SOL 7732-18-5 Water

RX(11) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)

RGT Q 7632-00-0 NaNO2

STAGE(3)

RGT G 7664-93-9 H2SO4

STAGE(4)

RCT AB 118-32-1
RGT R 144-55-8 NaHCO3
SOL 7732-18-5 Water

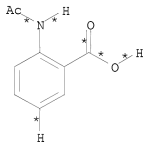
STAGE(5)

RGT S 7647-14-5 NaCl

PRO AC 315681-07-3

RX(87) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(12)

RX(87) A + B + J + AD ==> AE



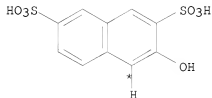
A



B



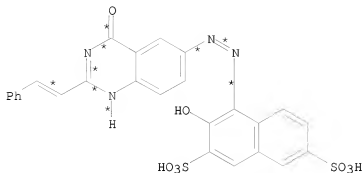
J



AD

● 2 Na

6
STEPS
→



• 2 Na

AE

YIELD 84%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3
RGT M 1313-82-2 Na2S
PRO L 30896-48-1
SOL 7732-18-5 Water

RX(12) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl

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SOL 7732-18-5 Water

STAGE(2)

RGT Q 7632-00-0 NaNO2

STAGE(3)

RGT G 7664-93-9 H2SO4

STAGE(4)

RCT AD 135-51-3

RGT R 144-55-8 NaHCO3

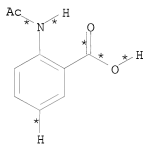
SOL 7732-18-5 Water

STAGE(5)

RGT S 7647-14-5 NaCl

PRO AE 315681-08-4

RX(88) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(13)
RX(88) A + B + J + AF ==> AG



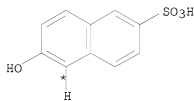
A



B

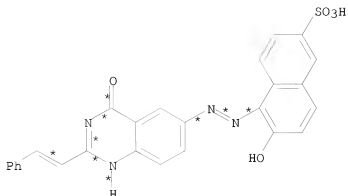


J



AF

6
STEPS
→



AG

YIELD 79%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3
RGT M 1313-82-2 Na2S
PRO L 30896-48-1
SOL 7732-18-5 Water

RX(13) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

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RGT Q 7632-00-0 NaNO2

STAGE(3)

RGT G 7664-93-9 H2SO4

STAGE(4)

RCT AF 93-01-6

RGT R 144-55-8 NaHCO3

SOL 7732-18-5 Water

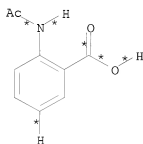
STAGE(5)

RGT S 7647-14-5 NaCl

PRO AG 315681-09-5

RX(89) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(14)

RX(89) A + B + J + AH ==> AI



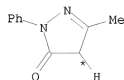
A



B

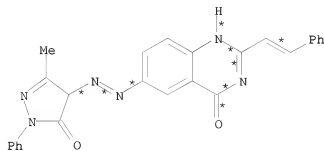


J



AH

6
STEPS
→



AI

YIELD 86%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

```

        STAGE(1)
          RGT  G 7664-93-9 H2SO4, H 7697-37-2 HNO3

        STAGE(2)
          SOL  7732-18-5 Water

    PRO  F 24688-36-6

RX(4)   RCT  F 24688-36-6

        STAGE(1)
          RGT  B 108-24-7 Ac2O

        STAGE(2)
          RCT  J 100-52-7

    PRO  K 24688-33-3

RX(5)   RCT  K 24688-33-3
        RGT  M 1313-82-2 Na2S
        PRO  L 30896-48-1
        SOL  7732-18-5 Water

RX(14)  RCT  L 30896-48-1

        STAGE(1)
          RGT  P 7647-01-0 HCl
          SOL  7732-18-5 Water

        STAGE(2)
          RGT  Q 7632-00-0 NaNO2

        STAGE(3)
          RGT  G 7664-93-9 H2SO4

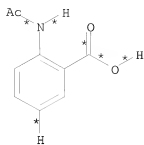
        STAGE(4)
          RCT  AH 89-25-8
          RGT  R 144-55-8 NaHCO3
          SOL  7732-18-5 Water

        STAGE(5)
          RGT  S 7647-14-5 NaCl

    PRO  AI 315681-10-8

RX(90) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(15)
RX(90)   A  +  B  +  J  +  AJ  ==>  AK

```



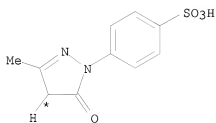
A



B

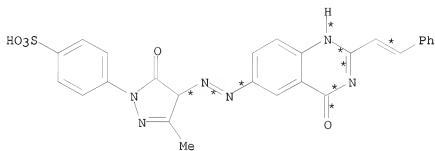


J



AJ

6
STEPS
→



AK

YIELD 81%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

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SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)
RGT B 108-24-7 Ac2O

STAGE(2)
RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3
RGT M 1313-82-2 Na2S
PRO L 30896-48-1
SOL 7732-18-5 Water

RX(15) RCT L 30896-48-1

STAGE(1)
RGT P 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)
RGT Q 7632-00-0 NaNO2

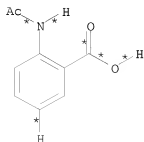
STAGE(3)
RGT G 7664-93-9 H2SO4

STAGE(4)
RCT AJ 89-36-1
RGT R 144-55-8 NaHCO3
SOL 7732-18-5 Water

STAGE(5)
RGT S 7647-14-5 NaCl

PRO AK 315681-11-9

RX(91) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(16)
RX(91) A + B + J + AL ==> AM



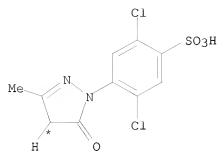
A



B

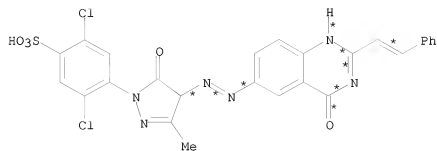


J



AL

6
STEPS
→



AM

YIELD 78%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

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RX(5) RCT K 24688-33-3
 RGT M 1313-82-2 Na2S
 PRO L 30896-48-1
 SOL 7732-18-5 Water

RX(16) RCT L 30896-48-1

STAGE(1)
 RGT P 7647-01-0 HCl
 SOL 7732-18-5 Water

STAGE(2)
 RGT Q 7632-00-0 NaNO2

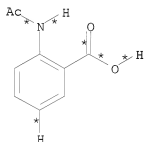
STAGE(3)
 RGT G 7664-93-9 H2SO4

STAGE(4)
 RCT AL 84-57-1
 RGT R 144-55-8 NaHCO3
 SOL 7732-18-5 Water

STAGE(5)
 RGT S 7647-14-5 NaCl

PRO AM 315681-12-0

RX(92) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(17)
 RX(92) A + B + J + AN ==> AO



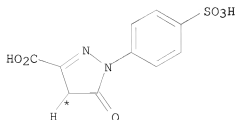
A



B

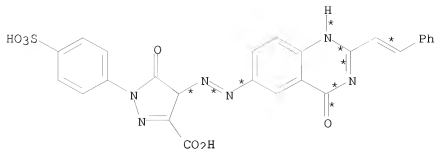


J



AN

6
 STEPS
 ==>



AO

YIELD 79%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3
RGT M 1313-82-2 Na2S
PRO L 30896-48-1
SOL 7732-18-5 Water

RX(17) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT Q 7632-00-0 NaNO2

STAGE(3)

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RGT G 7664-93-9 H2SO4

STAGE(4)

RCT AN 118-47-8

RGT R 144-55-8 NaHCO3

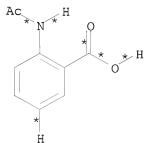
SOL 7732-18-5 Water

STAGE(5)

RGT S 7647-14-5 NaCl

PRO AO 315681-13-1

RX(93) OF 93 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(18)
RX(93) A + B + J + AP ==> AQ



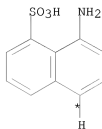
A



B

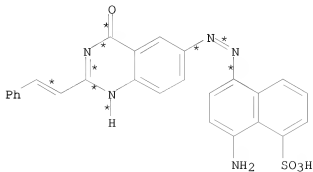


J



AP

6
STEPS
→



AQ
YIELD 78%

RX(1) RCT A 89-52-1, B 108-24-7
PRO C 525-76-8

RX(2) RCT C 525-76-8
RGT E 7664-41-7 NH3
PRO D 1769-24-0

RX(3) RCT D 1769-24-0

STAGE(1)

RGT G 7664-93-9 H2SO4, H 7697-37-2 HNO3

STAGE(2)

SOL 7732-18-5 Water

PRO F 24688-36-6

RX(4) RCT F 24688-36-6

STAGE(1)

RGT B 108-24-7 Ac2O

STAGE(2)

RCT J 100-52-7

PRO K 24688-33-3

RX(5) RCT K 24688-33-3

RGT M 1313-82-2 Na2S

PRO L 30896-48-1

SOL 7732-18-5 Water

RX(18) RCT L 30896-48-1

STAGE(1)

RGT P 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(2)

RGT Q 7632-00-0 NaNO2

STAGE(3)

RGT G 7664-93-9 H2SO4

STAGE(4)

RCT AP 82-75-7

RGT R 144-55-8 NaHCO3

SOL 7732-18-5 Water

STAGE(5)

RGT S 7647-14-5 NaCl

PRO AQ 315681-14-2

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 114 OF 258 CASREACT COPYRIGHT 2009 ACS on SIN

ACCESSION NUMBER: 134:4911 CASREACT

TITLE: Synthesis of quinazoline compound

AUTHOR(S): Shi, Qinqing; Liu, Zhiping

CORPORATE SOURCE: Shanghai Research Institute of Chemical Reagent,

Shanghai, 200333, Peop. Rep. China

SOURCE: Shanghai Huagong (2000), 25(9), 18-20

CODEN: SHAHE2; ISSN: 1004-017X

PUBLISHER: Shanghai Huagong Bianjibu

DOCUMENT TYPE: Journal

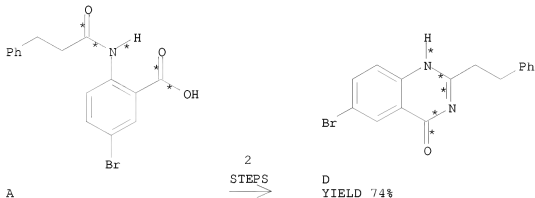
LANGUAGE:

Chinese

AB 6-Cyano-2-(2-phenylethyl)quinazolinone was prepared in 5 steps in 30.6% overall yield from 2-aminobenzoic acid.

RX(6) OF 15 COMPOSED OF RX(1), RX(2)

RX(6) A ==> D

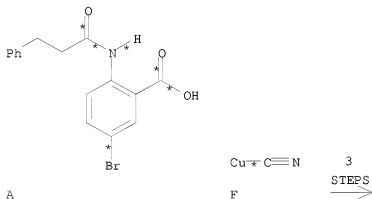


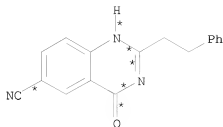
RX(1) RCT A 307001-06-5
 PRO B 307001-07-6
 SOL 108-24-7 Ac2O

RX(2) RCT B 307001-07-6
 RGT E 75-12-7 Formamide
 PRO D 307001-08-7

RX(10) OF 15 COMPOSED OF RX(1), RX(2), RX(3)

RX(10) A + F ==> G





G
YIELD 78%

RX(1) RCT A 307001-06-5
PRO B 307001-07-6
SOL 108-24-7 Ac2O

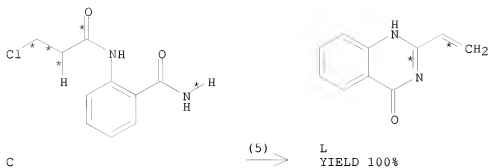
RX(2) RCT B 307001-07-6
RGT E 75-12-7 Formamide
PRO D 307001-08-7

RX(3) RCT F 544-92-3, D 307001-08-7
PRO G 307001-09-8
SOL 127-19-5 AcNMe2

L3 ANSWER 115 OF 258 CASREACT COPYRIGHT 2009 ACS on SIN
ACCESSION NUMBER: 133:362747 CASREACT
TITLE: Synthesis and Reactions of some
2-Vinyl-3H-quinazolin-4-ones
AUTHOR(S): Witt, A.; Bergman, J.
CORPORATE SOURCE: Department of Biosciences, Unit for Organic Chemistry,
Novum Research Park, Karolinska Institute and
Sodertorn University College, Huddinge, SE-141 57,
Swed.
SOURCE: Tetrahedron (2000), 56(37), 7245-7253
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

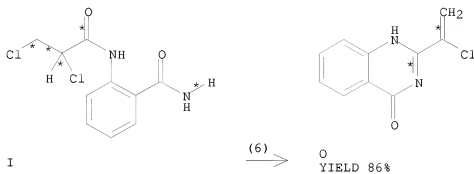
AB A simple, high-yielding synthesis of 2-vinyl-3H-quinazolin-4-one,
2-(1-chlorovinyl)-3H-quinazolin-4-one, and
2-(1-bromovinyl)-3H-quinazolin-4-one is reported. The
2-vinylquinazolinones participate readily in nucleophilic addition reactions.
Treatment with both carbon and nitrogen nucleophiles results in a clean
conversion into a variety of 2-substituted 3H-quinazolin-4-one derivs.
2-(1-Halovinyl)-3H-quinazolin-4-ones reacted with carbon nucleophiles to
give several derivs. of 2-substituted 3H-quinazolin-4-one.

RX(5) OF 72 ...C ==> L...



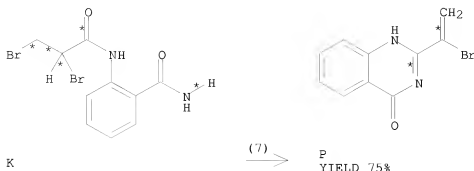
RX(5) RCT C 306996-53-2
RGT M 1310-73-2 NaOH
PRO L 91634-12-7
SOL 64-17-5 EtOH

RX(6) OF 72 ...I ==> O...



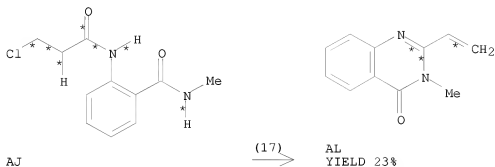
RX(6) RCT I 306996-54-3
RGT M 1310-73-2 NaOH
PRO O 306996-56-5
SOL 64-17-5 EtOH

RX(7) OF 72 ...K ==> P



RX (7) RCT K 306996-55-4
RGT M 1310-73-2 NaOH
PRO P 306996-57-6
SOL 64-17-5 EtOH

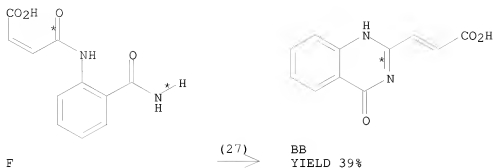
RX (17) OF 72 ...AJ ==> AL...



RX (17) RCT AJ 306996-58-7
RGT AM 497-19-8 Na2CO3
PRO AL 306996-59-8
SOL 67-56-1 MeOH

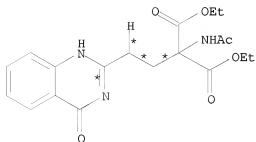
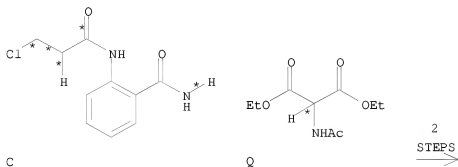
RX (27) OF 72 ...F ==> BB

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RX(27) RCT F 306996-83-8
RGT BC 127-09-3 AcONa
PRO BB 306996-85-0
SOL 108-24-7 Ac2O

RX(32) OF 72 COMPOSED OF RX(5), RX(8)
RX(32) C + Q ==> R



R
YIELD 80%

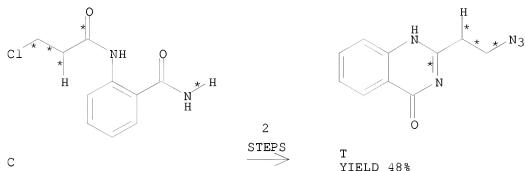
RX(5) RCT C 306996-53-2
RGT M 1310-73-2 NaOH
PRO L 91634-12-7

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SOL 64-17-5 EtOH

RX(8) RCT L 91634-12-7, Q 1068-90-2
 RGT S 7440-23-5 Na
 PRO R 306996-62-3
 SOL 64-17-5 EtOH

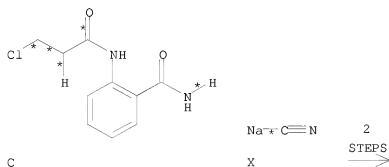
RX(33) OF 72 COMPOSED OF RX(5), RX(9)
 RX(33) C ==> T

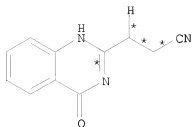


RX(5) RCT C 306996-53-2
 RGT M 1310-73-2 NaOH
 PRO L 91634-12-7
 SOL 64-17-5 EtOH

RX(9) RCT L 91634-12-7
 RGT U 26628-22-8 NaN₃
 PRO T 306996-66-7
 SOL 109-99-9 THF, 7732-18-5 Water

RX(34) OF 72 COMPOSED OF RX(5), RX(10)
 RX(34) C + X ==> Y



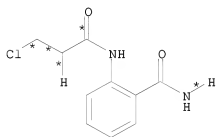


Y
YIELD 76%

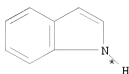
RX(5) RCT C 306996-53-2
RGT M 1310-73-2 NaOH
PRO L 91634-12-7
SOL 64-17-5 EtOH

RX(10) RCT L 91634-12-7, X 143-33-9
PRO Y 1703-02-2
SOL 64-17-5 EtOH, 7732-18-5 Water

RX(35) OF 72 COMPOSED OF RX(5), RX(21)
RX(35) C + AR ==> AS

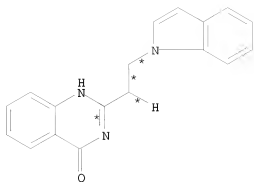


C



AR

2
STEPS
→



AS

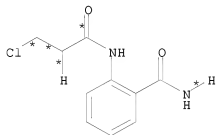
YIELD 95%

RX(5) RCT C 306996-53-2
 RGT M 1310-73-2 NaOH
 PRO L 91634-12-7
 SOL 64-17-5 EtOH

RX(21) RCT L 91634-12-7, AR 120-72-9
 PRO AS 306996-63-4
 SOL 64-19-7 AcOH

RX(36) OF 72 COMPOSED OF RX(5), RX(23)

RX(36) C + AV ==> AW



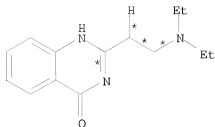
C



AV

2
 STEPS
 →

10/ 562,112



AW

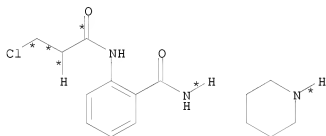
YIELD 49%

RX(5) RCT C 306996-53-2
 RGT M 1310-73-2 NaOH
 PRO L 91634-12-7
 SOL 64-17-5 EtOH

RX(23) RCT L 91634-12-7, AV 109-89-7
 RGT AT 64-19-7 AcOH
 PRO AW 95556-34-6
 SOL 67-56-1 MeOH

RX(37) OF 72 COMPOSED OF RX(5), RX(25)

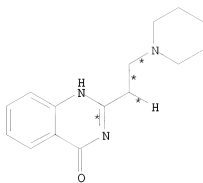
RX(37) C + AY ==> AZ



C

AY

2
 STEPS
 →



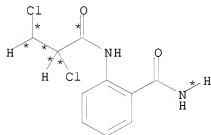
AZ

YIELD 84%

RX(5) RCT C 306996-53-2
 RGT M 1310-73-2 NaOH
 PRO L 91634-12-7
 SOL 64-17-5 EtOH

RX(25) RCT L 91634-12-7, AY 110-89-4
 RGT AT 64-19-7 AcOH
 PRO AZ 95698-00-3
 SOL 67-56-1 MeOH

RX(38) OF 72 COMPOSED OF RX(6), RX(11)
 RX(38) I + X ==> Z

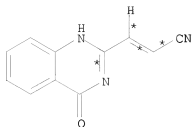


I



X

2
 STEPS
 →



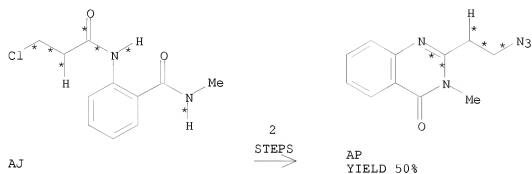
10/ 562,112

RX(17) RCT AJ 306996-58-7
 RGT AM 497-19-8 Na2CO3
 PRO AL 306996-59-8
 SOL 67-56-1 MeOH

RX(18) RCT AL 306996-59-8, Q 1068-90-2
 RGT AC 7646-69-7 NaH
 PRO AO 306996-69-0
 SOL 109-99-9 THF

RX(45) OF 72 COMPOSED OF RX(17), RX(19)

RX(45) AJ ==> AP

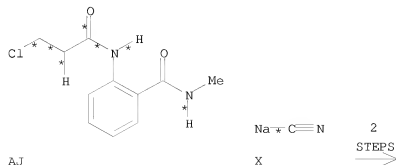


RX(17) RCT AJ 306996-58-7
 RGT AM 497-19-8 Na2CO3
 PRO AL 306996-59-8
 SOL 67-56-1 MeOH

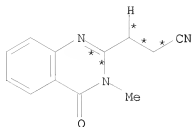
RX(19) RCT AL 306996-59-8
 RGT U 26628-22-8 NaN3
 PRO AP 306996-77-0
 SOL 109-99-9 THF, 7732-18-5 Water

RX(46) OF 72 COMPOSED OF RX(17), RX(20)

RX(46) AJ + X ==> AQ



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AQ

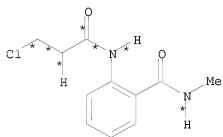
YIELD 23%

RX(17) RCT AJ 306996-58-7
 RGT AM 497-19-8 Na2CO3
 PRO AL 306996-59-8
 SOL 67-56-1 MeOH

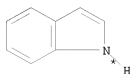
RX(20) RCT AL 306996-59-8, X 143-33-9
 PRO AQ 306996-79-2
 SOL 64-17-5 EtOH, 7732-18-5 Water

RX(47) OF 72 COMPOSED OF RX(17), RX(22)

RX(47) AJ + AR ==> AU

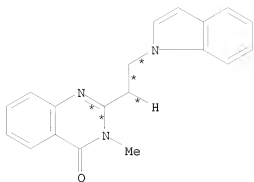


AJ



AR

2
 STEPS
 →



AU

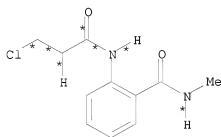
YIELD 75%

RX(17) RCT AJ 306996-58-7
 RGT AM 497-19-8 Na₂CO₃
 PRO AL 306996-59-8
 SOL 67-56-1 MeOH

RX(22) RCT AL 306996-59-8, AR 120-72-9
 PRO AU 306996-71-4
 SOL 64-19-7 AcOH

RX(48) OF 72 COMPOSED OF RX(17), RX(24)

RX(48) AJ + AV ==> AX

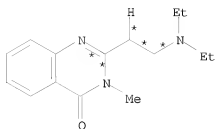


AJ



AV

2
 STEPS
 →



AX

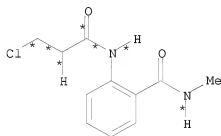
YIELD 85%

RX(17) RCT AJ 306996-58-7
 RGT AM 497-19-8 Na₂CO₃
 PRO AL 306996-59-8
 SOL 67-56-1 MeOH

RX(24) RCT AL 306996-59-8, AV 109-89-7
 RGT AT 64-19-7 AcOH
 PRO AX 306996-73-6
 SOL 67-56-1 MeOH

RX(49) OF 72 COMPOSED OF RX(17), RX(26)

RX(49) AJ + AY ==> BA

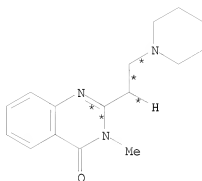


AJ



AY

2
 STEPS
 →



BA
YIELD 99%

RX(17) RCT AJ 306996-58-7
RGT AM 497-19-8 Na2CO3
PRO AL 306996-59-8
SOL 67-56-1 MeOH

RX(26) RCT AL 306996-59-8, AY 110-89-4
RGT AT 64-19-7 AcOH
PRO BA 306996-75-8
SOL 67-56-1 MeOH

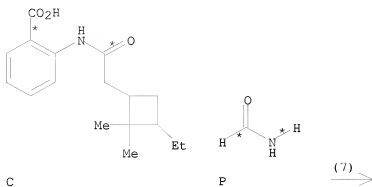
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 116 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 132:180542 CASREACT
TITLE: 2-[(3-Ethyl-2,2-dimethylcyclobutyl)methyl]-4(3H)-quinazolinones
AUTHOR(S): Avotin'sh, F. M.; Petrova, M. V.; Pastors, P. V.; Strakov, A. Ya.
CORPORATE SOURCE: Riga Technical University, Riga, LV-1658, Latvia
SOURCE: Chemistry of Heterocyclic Compounds (New York) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (1999), 35(6), 722-728
CODEN: CHCCAL; ISSN: 0009-3122
PUBLISHER: Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Anthranilic acid and its 5-bromo and 4-chloro derivs. react with pinanoic and pinonoic acid chlorides to give the corresponding N-acyl derivs. The pinanoyl derivs. give the title compds. when refluxed in formamide. Pinanoylanthranilic acid reacts with dicyclohexylcarbodiimide to give 2-[(3-ethyl-2,2-dimethylcyclobutyl)methyl]benz-3,1-oxazin-4(H)-one and subsequently with hydrazine hydrate to give 3-amino-2-[(3-ethyl-2,2-dimethylcyclobutyl)methyl]-4(3H)-quinazolinone. Refluxing the pinanoyl- and pinonoylanthranilic acids with acetic anhydride gives acetylanthranilic acid, and pinonoylanthranilic acid gives 4(3H)-quinazolinone with formamide.

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RX(7) OF 22 ...C + P ==> Q



Q
YIELD 70%

RX(7) RCT C 259262-82-3, P 75-12-7

STAGE(1)

STAGE(2)

RGT R 144-55-8 NaHCO3

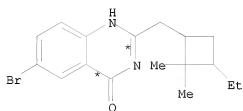
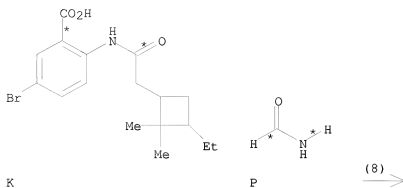
SOL 7732-18-5 Water

PRO Q 259262-90-3

NTE first stage thermal without solvent

RX(8) OF 22 ...K + P ==> S

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S
YIELD 93%

RX(8) RCT K 259262-83-4, P 75-12-7

STAGE(1)

STAGE(2)

RGT R 144-55-8 NaHCO₃

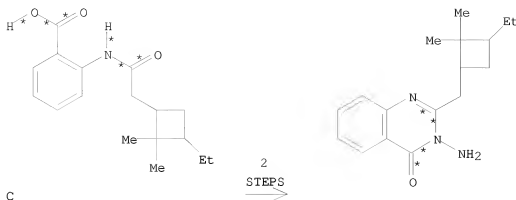
SOL 7732-18-5 Water

PRO S 259262-91-4

NTE first stage thermal without solvent

RX(20) OF 22 COMPOSED OF RX(12), RX(13)

RX(20) C ==> AB



● HCl

AB
YIELD 63%

RX(12) RCT C 259262-82-3
RGT AA 538-75-0 DCC
PRO Z 259262-93-6
SOL 71-43-2 Benzene

RX(13) RCT Z 259262-93-6

STAGE(1)

RGT AC 302-01-2 N₂H₄
SOL 110-86-1 Pyridine

STAGE(2)

RGT E 7647-01-0 HCl
SOL 7732-18-5 Water

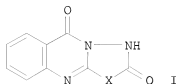
PRO AB 259262-94-7

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 117 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 131:286478 CASREACT
TITLE: Transformations of diacyl derivatives of anthranilic hydrazide under cyclodehydration conditions
AUTHOR(S): Shemchuk, L. A.; Chernykh, V. P.; Ivanova, I. L.; Snitkovskii, E. L.; Zhiron, M. V.; Turov, A. V.
CORPORATE SOURCE: Ukrainian Pharmaceutical Academy, Kharkov, 10002, Ukraine
SOURCE: Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (1999), 35(2), 286-289
CODEN: RJOCEQ; ISSN: 1070-4280
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal

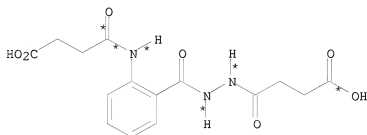
LANGUAGE:
GI

English



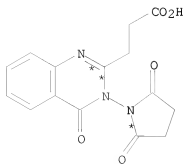
AB Acylation of anthranilic hydrazide with anhydrides of dicarboxylic acids afforded succinic N'-[2-(3-carboxypropionylamino)benzoyl]hydrazide, glutaric N'-[2-(4-carboxybutyrylamino)benzoyl]hydrazide, and phthalic N'-[2-(2-carboxybenzoylamino)benzoyl]hydrazide. Heating these compds. in acetic anhydride with sodium acetate yielded the corresponding diimides. Thermolysis of the diacyl derivs. of the anthranilic hydrazides containing succinic and phthalic moieties furnished, resp., 3,4-dihydropyridazino[2,3-b]quinazoline-2,10-dione (I, X = CH₂CH₂) and phthalazino[1,2-b]quinazoline-2,12-dione (I, X = o-C₆H₄). In acetic acid diimides or derivs. of 4-quinazolinone were formed, depending on the nature of the dicarboxylic acid.

RX(11) OF 18 ...C ==> T



C

(11) →

T
YIELD 51%

RX(11) RCT C 245724-38-3

STAGE(1)

RGT O 64-19-7 AcOH

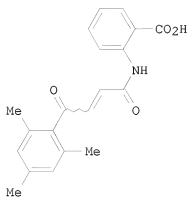
STAGE(2)

RGT L 7732-18-5 Water

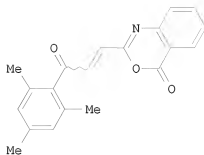
PRO T 245724-45-2

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

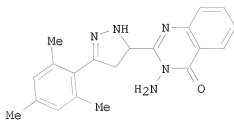
L3 ANSWER 118 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 131:129961 CASREACT
TITLE: Synthesis and reactions of
2-[2-(2,4,6-trimethylbenzoyl)vinyl]-4H-3,1-benzoxazin-
4-one and antimicrobial activity
AUTHOR(S): Abdel-Fattah, M. E.; Soliman, E. A.; Soliman, S. M. A.
CORPORATE SOURCE: Chemistry Department, Faculty of Science, Suez Canal
University Ismailia, Cairo, Egypt
SOURCE: Indian Journal of Heterocyclic Chemistry (1999), 8(3),
177-182
CODEN: IJCHEI; ISSN: 0971-1627
PUBLISHER: Prof. R. S. Varma
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



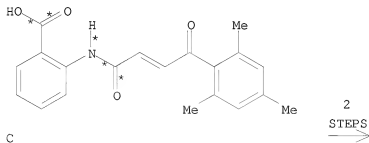
II



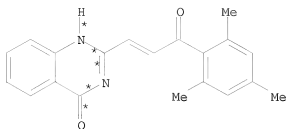
III

AB β -(2,4,6-Trimethylbenzoyl)-acryloyl chloride reacts with anthranilic acid to give adduct I which is cyclized by the action of acetic anhydride to give the benzoxazinone II. Condensation of II with hydrazine hydrate gave pyrazole III. The behavior of III towards aromatic aldehydes, ketones, phthalic Anhydride, and amino acid chlorides has been investigated. Reaction of II with o-phenylenediamine, ammonia, Grignard reagents, Friedel-Crafts reaction and bromine has been described. Some of the compds. were tested for antibacterial activity; some were active against gram-neg. and gram-pos. bacterial.

RX(31) OF 87 COMPOSED OF RX(2), RX(6)
RX(31) C ==> O



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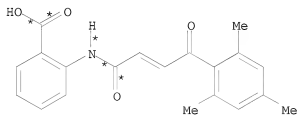


O

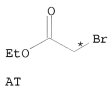
RX(2) RCT C 234103-28-7
 PRO E 234103-30-1
 SOL 108-24-7 Ac2O

RX(6) RCT E 234103-30-1
 RGT P 7664-41-7 NH3
 PRO O 234103-64-1
 SOL 64-17-5 EtOH

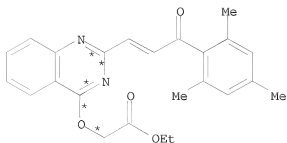
RX(72) OF 87 COMPOSED OF RX(2), RX(6), RX(21)
 RX(72) C + AT ==> AU



C



3
 STEPS
 →



AU

RX(2) RCT C 234103-28-7
 PRO E 234103-30-1
 SOL 108-24-7 Ac2O

RX(6) RCT E 234103-30-1
 RGT P 7664-41-7 NH3
 PRO O 234103-64-1
 SOL 64-17-5 EtOH

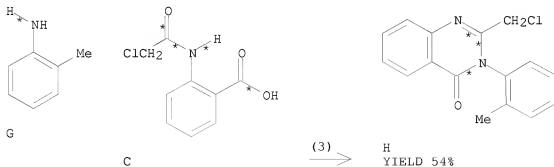
RX(21) RCT O 234103-64-1, AT 105-36-2
 RGT AV 584-08-7 K2CO3
 PRO AU 234103-66-3
 SOL 67-64-1 Me2CO

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 119 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 130:311760 CASREACT
 TITLE: Synthesis and fungicidal activity of 3-aryl-2-(4'-arylthiazol-2'-ylaminomethyl) quinazol-4 (3H)-ones
 AUTHOR(S): Pattanaik, J. M.; Pattanaik, M.; Bhatta, D.
 CORPORATE SOURCE: Department of Chemistry, Utkal University, Bhubaneswar, 751 004, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1998), 37B(12), 1304-1306
 CODEN: IJSBDB; ISSN: 0376-4699
 PUBLISHER: National Institute of Science Communication, CSIR
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A series of 3-aryl-2-(4-aryl-2-thiazolylaminomethyl) quinazol-4(3H)-ones was prepared by condensing 3-aryl-2-chloromethylquinazol-4(3H)-ones with 2-amino-4-substituted phenylthiazoles. Another group of 3-aryl-6,8-dibromo-2-(4-aryl-2-thiazolylaminomethyl)quinazol-4(3H)-ones was also synthesized from 3-aryl-6,8-dibromo-2-chloromethylquinazol-4(3H)-ones and 2-amino-4-substituted phenylthiazoles in the same manner. Their antifungal activity was determined

RX(3) OF 106 ...G + C ==> H...

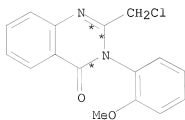
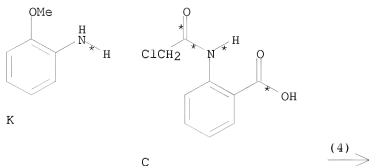


RX(3) RCT G 95-53-4, C 14422-49-2
 RGT I 584-08-7 K2CO3
 PRO H 3166-54-9

10/ 562,112

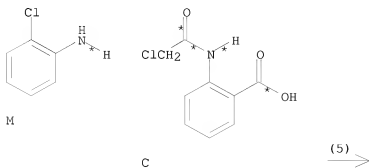
SOL 64-17-5 EtOH
NTE 6 H

RX(4) OF 106 ...K + C ==> L...

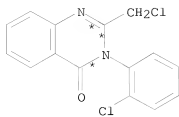


RX(4) RCT K 90-04-0, C 14422-49-2
RGT I 584-08-7 K2CO3
PRO L 22312-81-8
SOL 64-17-5 EtOH
NTE 6 H

RX(5) OF 106 ...M + C ==> N...



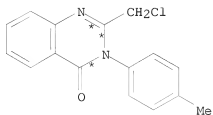
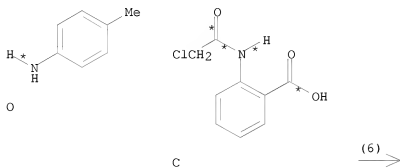
10/ 562,112



N
YIELD 54%

RX(5) RCT M 95-51-2, C 14422-49-2
 RGT I 584-08-7 K2CO3
 PRO N 22312-83-0
 SOL 64-17-5 EtOH
 NTE 6 H

RX(6) OF 106 ...O + C ==> P...



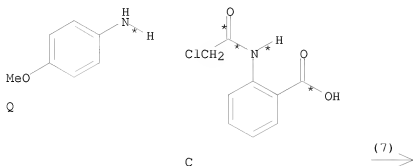
P
YIELD 54%

RX(6) RCT O 106-49-0, C 14422-49-2
 RGT I 584-08-7 K2CO3
 PRO P 22312-80-7

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SOL 64-17-5 EtOH
NTE 6 H

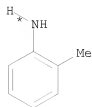
RX(7) OF 106 ...Q + C ==> R...



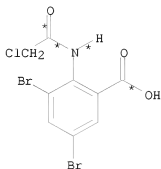
R
YIELD 54%

RX(7) RCT Q 104-94-9, C 14422-49-2
RGT I 584-08-7 K2CO3
PRO R 22312-82-9
SOL 64-17-5 EtOH
NTE 6 H

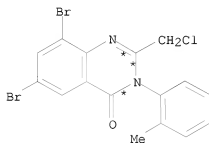
RX(8) OF 106 ...G + F ==> S...



G



F

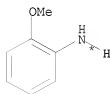
(8) \longrightarrow 

S

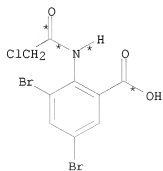
YIELD 59%

RX(8) RCT G 95-53-4, F 103952-88-1
 RGT I 584-08-7 K2CO3
 PRO S 177167-07-6
 SOL 64-17-5 EtOH
 NTE 6 H

RX(9) OF 106 ...K + F ==> T...

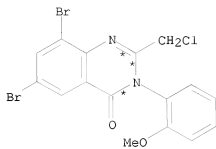


K



F

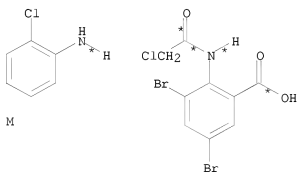
(9) \longrightarrow



T
YIELD 54%

RX(9) RCT K 90-04-0, F 103952-88-1
 RGT I 584-08-7 K2CO3
 PRO T 104308-99-8
 SOL 64-17-5 EtOH
 NTE 6 H

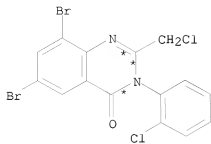
RX(10) OF 106 ...M + F ==> U...



F

(10) →

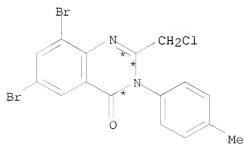
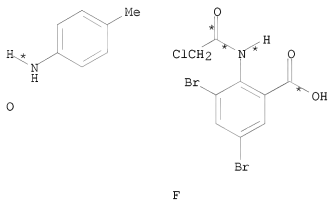
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U
YIELD 54%

RX(10) RCT M 95-51-2, F 103952-88-1
 RGT I 584-08-7 K2CO3
 PRO U 104308-98-7
 SOL 64-17-5 EtOH
 NTE 6 H

RX(11) OF 106 ...O + F ==> V...

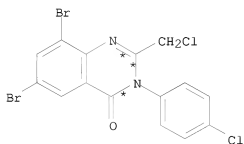
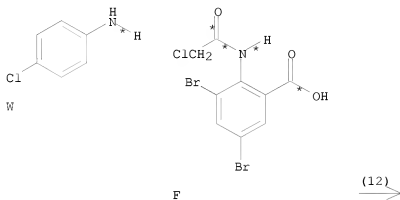


V
YIELD 54%

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RX(11) RCT O 106-49-0, F 103952-88-1
RGT I 584-08-7 K2CO3
PRO V 103952-89-2
SOL 64-17-5 EtOH
NTE 6 H

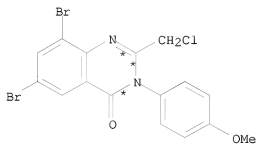
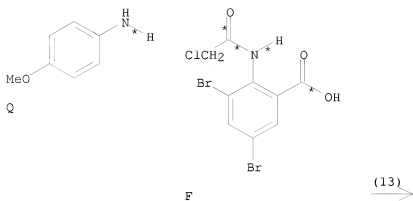
RX(12) OF 106 ...W + F ==> X...



X
YIELD 54%

RX(12) RCT W 106-47-8, F 103952-88-1
RGT I 584-08-7 K2CO3
PRO X 223590-80-5
SOL 64-17-5 EtOH
NTE 6 H

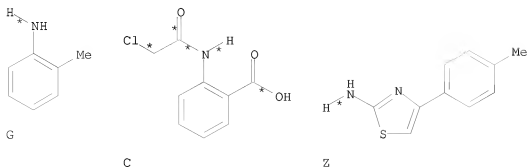
RX(13) OF 106 ...Q + F ==> Y...



Y
YIELD 54%

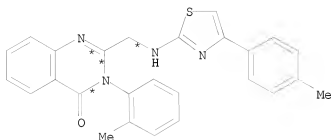
RX(13) RCT Q 104-94-9, F 103952-88-1
 RGT I 584-08-7 K2CO3
 PRO Y 223590-81-6
 SOL 64-17-5 EtOH
 NTE 6 H

RX(57) OF 106 COMPOSED OF RX(3), RX(16)
 RX(57) G + C + Z ==> AE



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2
STEPS
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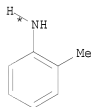


AE
YIELD 56%

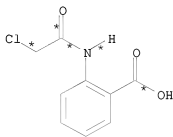
RX(3) RCT G 95-53-4, C 14422-49-2
RGT I 584-08-7 K2CO3
PRO H 3166-54-9
SOL 64-17-5 EtOH
NTE 6 H

RX(16) RCT Z 2103-91-5, H 3166-54-9
RGT B 110-86-1 Pyridine
PRO AE 223590-50-9
NTE 4 H

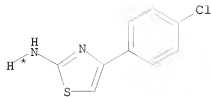
RX(58) OF 106 COMPOSED OF RX(3), RX(17)
RX(58) G + C + AC ==> AF



G

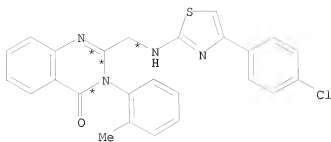


C



AC

2
STEPS
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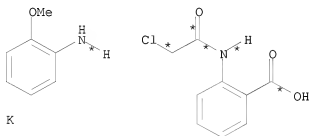


AF
YIELD 49%

RX(3) RCT G 95-53-4, C 14422-49-2
RGT I 584-08-7 K2CO3
PRO H 3166-54-9
SOL 64-17-5 EtOH
NTE 6 H

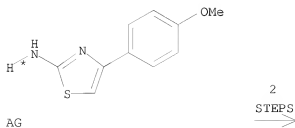
RX(17) RCT AC 2103-99-3, H 3166-54-9
RGT B 110-86-1 Pyridine
PRO AF 223590-51-0
NTE 4 H

RX(59) OF 106 COMPOSED OF RX(4), RX(18)
RX(59) K + C + AG ==> AH



K

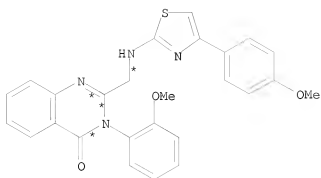
C



AG

2
STEPS
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AH

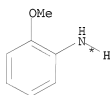
YIELD 52%

RX(4) RCT K 90-04-0, C 14422-49-2
 RGT I 584-08-7 K2CO3
 PRO L 22312-81-8
 SOL 64-17-5 EtOH
 NTE 6 H

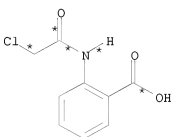
RX(18) RCT AG 2104-04-3, L 22312-81-8
 RGT B 110-86-1 Pyridine
 PRO AH 223590-52-1
 NTE 4 H

RX(60) OF 106 COMPOSED OF RX(4), RX(19)

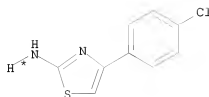
RX(60) K + C + AC ==> AI



K



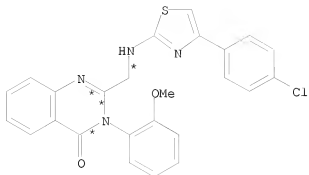
C



AC

2
 STEPS
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AI

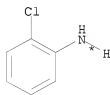
YIELD 60%

RX(4) RCT K 90-04-0, C 14422-49-2
 RGT I 584-08-7 K2CO3
 PRO L 22312-81-8
 SOL 64-17-5 EtOH
 NTE 6 H

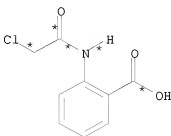
RX(19) RCT AC 2103-99-3, L 22312-81-8
 RGT B 110-86-1 Pyridine
 PRO AI 223590-53-2
 NTE 4 H

RX(61) OF 106 COMPOSED OF RX(5), RX(20)

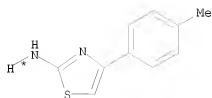
RX(61) M + C + Z ==> AJ



M

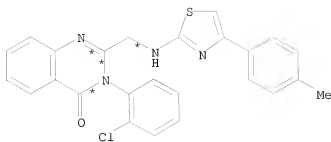


C



Z

2
 STEPS
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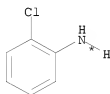


AJ
YIELD 56%

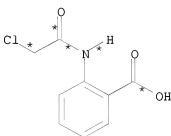
RX(5) RCT M 95-51-2, C 14422-49-2
RGT I 584-08-7 K2CO3
PRO N 22312-83-0
SOL 64-17-5 EtOH
NTE 6 H

RX(20) RCT Z 2103-91-5, N 22312-83-0
RGT B 110-86-1 Pyridine
PRO AJ 223590-54-3
NTE 4 H

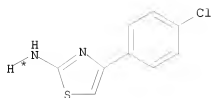
RX(62) OF 106 COMPOSED OF RX(5), RX(21)
RX(62) M + C + AC ==> AK



M



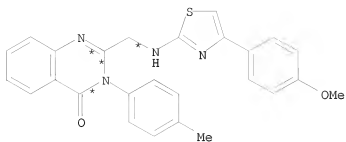
C



AC

2
STEPS
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AM

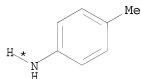
YIELD 52%

RX(6) RCT O 106-49-0, C 14422-49-2
 RGT I 584-08-7 K2CO3
 PRO P 22312-80-7
 SOL 64-17-5 EtOH
 NTE 6 H

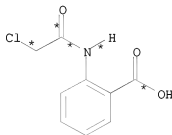
RX(23) RCT AG 2104-04-3, P 22312-80-7
 RGT B 110-86-1 Pyridine
 PRO AM 223590-57-6
 NTE 4 H

RX(65) OF 106 COMPOSED OF RX(6), RX(24)

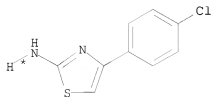
RX(65) O + C + AC ==> AN



O



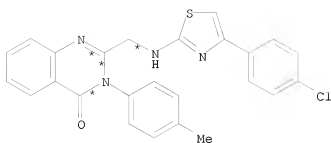
C



AC

2
 STEPS
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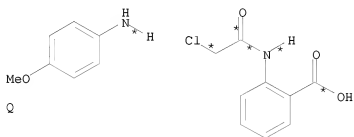


AN
YIELD 48%

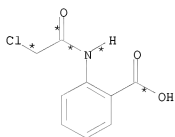
RX(6) RCT O 106-49-0, C 14422-49-2
RGT I 584-08-7 K2CO3
PRO P 22312-80-7
SOL 64-17-5 EtOH
NTE 6 H

RX(24) RCT AC 2103-99-3, P 22312-80-7
RGT B 110-86-1 Pyridine
PRO AN 223590-58-7
NTE 4 H

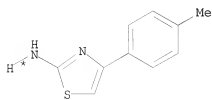
RX(66) OF 106 COMPOSED OF RX(7), RX(28)
RX(66) Q + C + Z ==> AS



Q

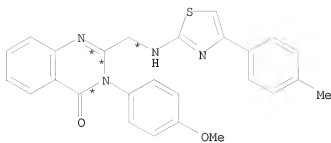


C



Z

2
STEPS
→



AS

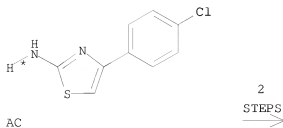
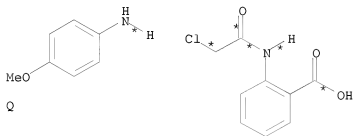
YIELD 51%

RX(7) RCT Q 104-94-9, C 14422-49-2
 RGT I 584-08-7 K2CO3
 PRO R 22312-82-9
 SOL 64-17-5 EtOH
 NTE 6 H

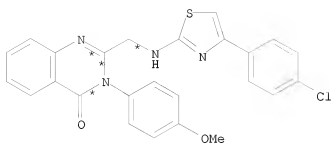
RX(28) RCT Z 2103-91-5, R 22312-82-9
 RGT B 110-86-1 Pyridine
 PRO AS 223590-62-3
 NTE 4 H

RX(67) OF 106 COMPOSED OF RX(7), RX(29)

RX(67) Q + C + AC ==> AT



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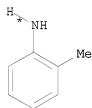


AT
YIELD 62%

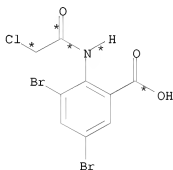
RX(7) RCT Q 104-94-9, C 14422-49-2
RGT I 584-08-7 K2CO3
PRO R 22312-82-9
SOL 64-17-5 EtOH
NTE 6 H

RX(29) RCT AC 2103-99-3, R 22312-82-9
RGT B 110-86-1 Pyridine
PRO AT 223590-63-4
NTE 4 H

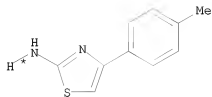
RX(68) OF 106 COMPOSED OF RX(8), RX(32)
RX(68) G + F + Z ==> AX



G



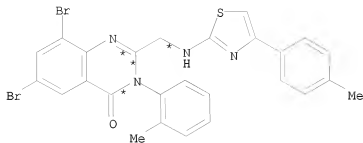
F



Z

2
STEPS
→

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AX

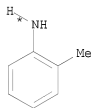
YIELD 54%

RX(8) RCT G 95-53-4, F 103952-88-1
 RGT I 584-08-7 K2CO3
 PRO S 177167-07-6
 SOL 64-17-5 EtOH
 NTE 6 H

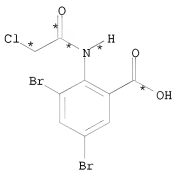
RX(32) RCT Z 2103-91-5, S 177167-07-6
 RGT B 110-86-1 Pyridine
 PRO AX 223590-66-7
 NTE 4 H

RX(69) OF 106 COMPOSED OF RX(8), RX(33)

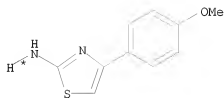
RX(69) G + F + AG ==> AY



G



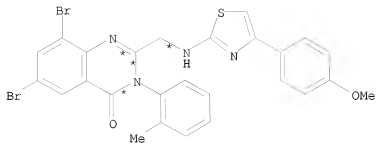
F



AG

2
 STEPS
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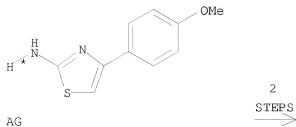
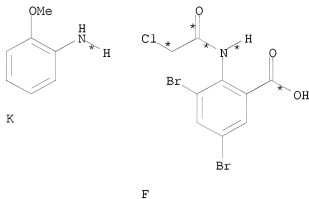


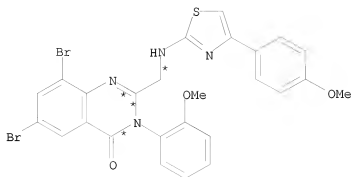
AY
YIELD 54%

RX(8) RCT G 95-53-4, F 103952-88-1
RGT I 584-08-7 K2CO3
PRO S 177167-07-6
SOL 64-17-5 EtOH
NTE 6 H

RX(33) RCT AG 2104-04-3, S 177167-07-6
RGT B 110-86-1 Pyridine
PRO AY 223590-67-8
NTE 4 H

RX(70) OF 106 COMPOSED OF RX(9), RX(34)
RX(70) K + F + AG ==> AZ



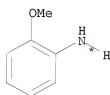


AZ
YIELD 56%

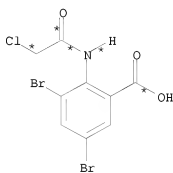
RX(9) RCT K 90-04-0, F 103952-88-1
RGT I 584-08-7 K2CO3
PRO T 104308-99-8
SOL 64-17-5 EtOH
NTE 6 H

RX(34) RCT AG 2104-04-3, T 104308-99-8
RGT B 110-86-1 Pyridine
PRO AZ 223590-68-9
NTE 4 H

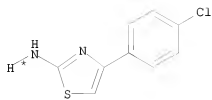
RX(71) OF 106 COMPOSED OF RX(9), RX(35)
RX(71) K + F + AC ==> BA



K

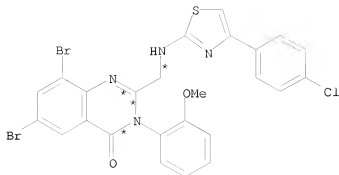


F



AC

2
STEPS
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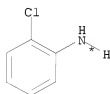


BA
YIELD 57%

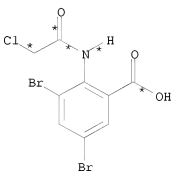
RX(9) RCT K 90-04-0, F 103952-88-1
RGT I 584-08-7 K2CO3
PRO T 104308-99-8
SOL 64-17-5 EtOH
NTE 6 H

RX(35) RCT AC 2103-99-3, T 104308-99-8
RGT B 110-86-1 Pyridine
PRO BA 223590-69-0
NTE 4 H

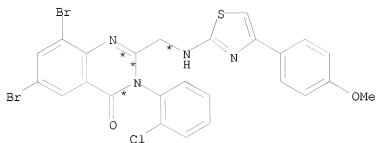
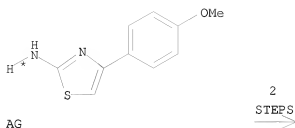
RX(72) OF 106 COMPOSED OF RX(10), RX(36)
RX(72) M + F + AG ==> BB



M



F

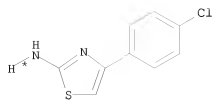
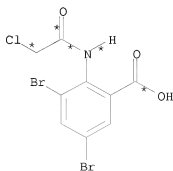
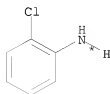


YIELD 48%

RX(10) RCT M 95-51-2, F 103952-88-1
RGT I 584-08-7 K2CO3
PRO U 104308-98-7
SOL 64-17-5 EtOH
NTE 6 H

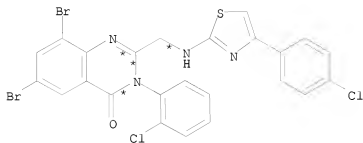
RX(36) RCT AG 2104-04-3, U 104308-98-7
RGT B 110-86-1 Pyridine
PRO BB 223590-70-3
NTE 4 H

RX(73) OF 106 COMPOSED OF RX(10), RX(37)
RX(73) M + F + AC ==> BC



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2
STEPS
→

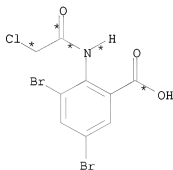
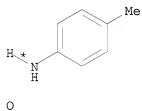


BC
YIELD 51%

RX(10) RCT M 95-51-2, F 103952-88-1
RGT I 584-08-7 K2CO3
PRO U 104308-98-7
SOL 64-17-5 EtOH
NTE 6 H

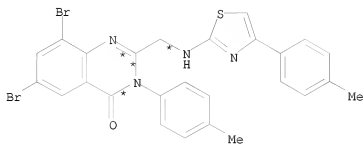
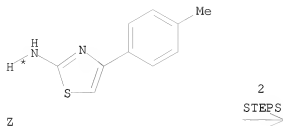
RX(37) RCT AC 2103-99-3, U 104308-98-7
RGT B 110-86-1 Pyridine
PRO BC 223590-71-4
NTE 4 H

RX(74) OF 106 COMPOSED OF RX(11), RX(38)
RX(74) O + F + Z ==> BD



F

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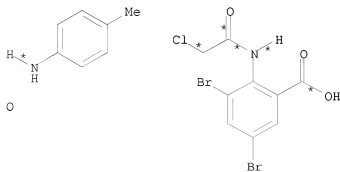


BD
YIELD 59%

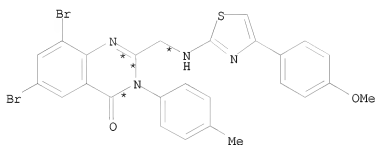
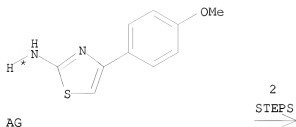
RX(11) RCT O 106-49-0, F 103952-88-1
RGT I 584-08-7 K2CO3
PRO V 103952-89-2
SOL 64-17-5 EtOH
NTE 6 H

RX(38) RCT Z 2103-91-5, V 103952-89-2
RGT B 110-86-1 Pyridine
PRO BD 223590-72-5
NTE 4 H

RX(75) OF 106 COMPOSED OF RX(11), RX(39)
RX(75) O + F + AG ==> BE



F

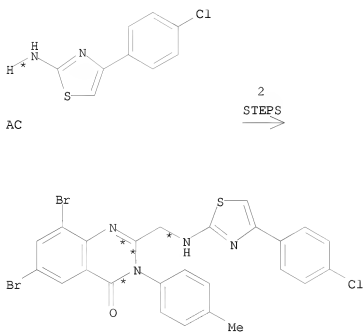
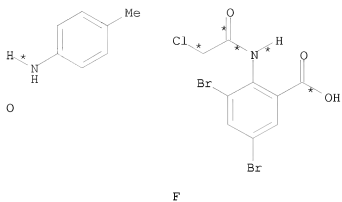


BE
YIELD 49%

RX(11) RCT O 106-49-0, F 103952-88-1
 RGT I 584-08-7 K2CO3
 PRO V 103952-89-2
 SOL 64-17-5 EtOH
 NTE 6 H

RX(39) RCT AG 2104-04-3, V 103952-89-2
 RGT B 110-86-1 Pyridine
 PRO BE 223590-73-6
 NTE 4 H

RX(76) OF 106 COMPOSED OF RX(11), RX(40)
 RX(76) O + F + AC ==> BF



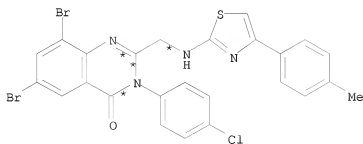
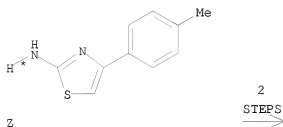
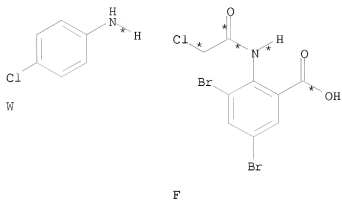
YIELD 60%

RX(11) RCT O 106-49-0, F 103952-88-1
 RGT I 584-08-7 K2CO3
 PRO V 103952-89-2
 SOL 64-17-5 EtOH
 NTE 6 H

RX(40) RCT AC 2103-99-3, V 103952-89-2
 RGT B 110-86-1 Pyridine
 PRO BF 223590-74-7
 NTE 4 H

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RX(77) OF 106 COMPOSED OF RX(12), RX(41)
 RX(77) W + F + Z ==> BG

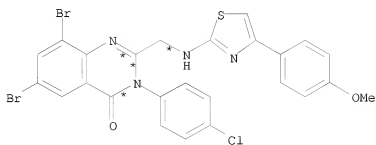
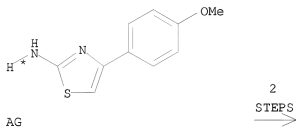
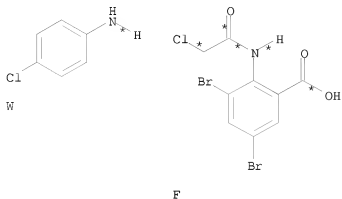


BG
 YIELD 47%

RX(12) RCT W 106-47-8, F 103952-88-1
 RGT I 584-08-7 K2CO3
 PRO X 223590-80-5
 SOL 64-17-5 EtOH
 NTE 6 H

RX(41) RCT Z 2103-91-5, X 223590-80-5
 RGT B 110-86-1 Pyridine
 PRO BG 223590-75-8
 NTE 4 H

RX(78) OF 106 COMPOSED OF RX(12), RX(42)
 RX(78) W + F + AG ==> BH



BH
 YIELD 56%

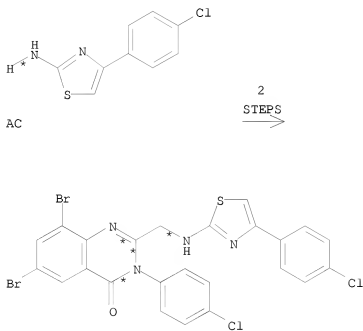
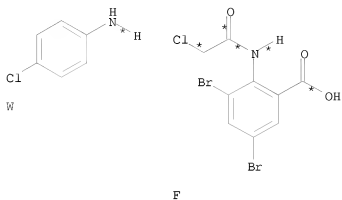
RX(12) RCT W 106-47-8, F 103952-88-1
 RGT I 584-08-7 K2CO3
 PRO X 223590-80-5
 SOL 64-17-5 EtOH
 NTE 6 H

RX(42) RCT AG 2104-04-3, X 223590-80-5
 RGT B 110-86-1 Pyridine

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PRO BH 223590-76-9
NTE 4 H

RX(79) OF 106 COMPOSED OF RX(12), RX(43)
RX(79) W + F + AC ==> BI



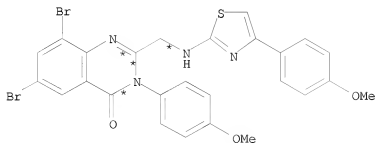
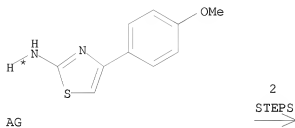
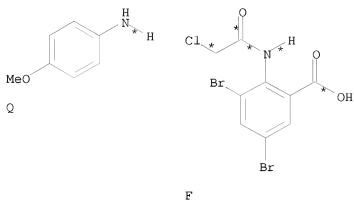
BI
YIELD 59%

RX(12) RCT W 106-47-8, F 103952-88-1
RGT I 584-08-7 K2CO3
PRO X 223590-80-5
SOL 64-17-5 EtOH
NTE 6 H

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RX(43) RCT AC 2103-99-3, X 223590-80-5
RGT B 110-86-1 Pyridine
PRO BI 223590-77-0
NTE 4 H

RX(80) OF 106 COMPOSED OF RX(13), RX(44)
RX(80) Q + F + AG ==> BJ



BJ
YIELD 53%

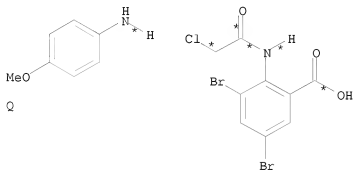
RX(13) RCT Q 104-94-9, F 103952-88-1
RGT I 584-08-7 K2CO3
PRO Y 223590-81-6
SOL 64-17-5 EtOH

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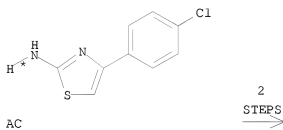
NTE 6 H

RX(44) RCT AG 2104-04-3, Y 223590-81-6
RGT B 110-86-1 Pyridine
PRO BJ 223590-78-1
NTE 4 H

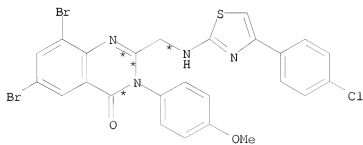
RX(81) OF 106 COMPOSED OF RX(13), RX(45)
RX(81) Q + F + AC ==> BK



F



AC



BK
YIELD 51%

RX(13) RCT Q 104-94-9, F 103952-88-1
RGT I 584-08-7 K₂CO₃

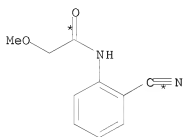
PRO Y 223590-81-6
 SOL 64-17-5 EtOH
 NTE 6 H

RX(45) RCT AC 2103-99-3, Y 223590-81-6
 RGT B 110-86-1 Pyridine
 PRO BK 223590-79-2
 NTE 4 H

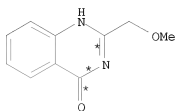
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 120 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 130:110232 CASREACT
 TITLE: A facile route to quinazolin-4(3H)-ones functionalized at the 2-position
 AUTHOR(S): Bavetsias, V.
 CORPORATE SOURCE: CRC Laboratory, CRC Centre for Cancer Therapeutics at The Institute of Cancer Research, Surrey, SM2 5NG, UK
 SOURCE: Synthetic Communications (1998), 28(24), 4547-4559
 CODEN: SYNCAV; ISSN: 0039-7911
 PUBLISHER: Marcel Dekker, Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Treatment of 2-methoxyacetamidobenzonitriles or 2-chloroacetamidobenzonitrile with UHP and K2CO3 provides a convenient route to 2-methoxymethyl- or 2-chloromethylquinazolin-4(3H)-ones. In addition, demethylation of 2-methoxymethylquinazolin-4(3H)-ones with 48% HBr gives 2-hydroxymethylquinazolin-4(3H)-ones.

RX(1) OF 12 A ==> B...



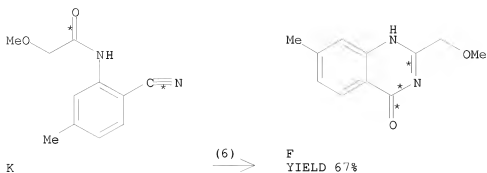
A



B
 YIELD 67%

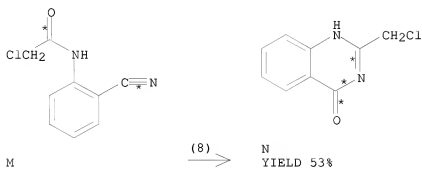
RX(1) RCT A 219739-45-4
 PRO B 21721-76-6
 SOL 67-64-1 Me2CO
 NTE 50 H, 82.deg.

RX(6) OF 12 K ==> F...



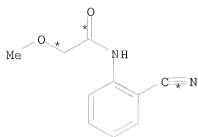
RX(6) RCT K 219739-46-5
 PRO F 219739-48-7
 SOL 67-64-1 Me2CO
 NTE 46 H, 82.deg.

RX(8) OF 12 M ==> N



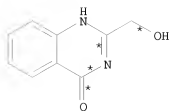
RX(8) RCT M 71993-21-0
 PRO N 3817-05-8
 SOL 67-64-1 Me2CO
 NTE 30 H, 84.deg.

RX(9) OF 12 COMPOSED OF RX(1), RX(2)
 RX(9) A ==> D



A

2
STEPS
→

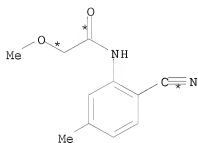


D
YIELD 61%

RX(1) RCT A 219739-45-4
PRO B 21721-76-6
SOL 67-64-1 Me2CO
NTE 50 H, 82.deg.

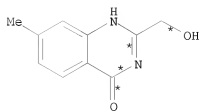
RX(2) RCT B 21721-76-6
RGT E 10035-10-6 HBr
PRO D 34637-40-6
NTE 11 H, 120.deg.

RX(10) OF 12 COMPOSED OF RX(6), RX(3)
RX(10) K ==> G



K

2
STEPS
→



G
YIELD 61%

RX(6) RCT K 219739-46-5
PRO F 219739-48-7
SOL 67-64-1 Me2CO
NTE 46 H, 82.deg.

RX(3) RCT F 219739-48-7
RGT E 10035-10-6 HBr
PRO G 219739-50-1
NTE 6 H, 120.deg.

RX(11) OF 12 COMPOSED OF RX(6), RX(4)
RX(11) K ==> H



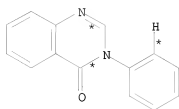
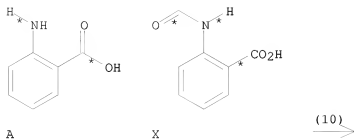
RX(6) RCT K 219739-46-5
 PRO F 219739-48-7
 SOL 67-64-1 Me2CO
 NTE 46 H, 82.deg.

RX(4) RCT F 219739-48-7
 RGT E 10035-10-6 HBr
 PRO H 219739-51-2
 NTE 6 H, 120.deg.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 121 OF 258 CASREACT COPYRIGHT 2009 ACS on SIN
 ACCESSION NUMBER: 130:81480 CASREACT
 TITLE: One-pot synthesis of substituted quinazolin-4(3H)-ones under microwave irradiation
 AUTHOR(S): Rad-Moghadam, Kurosh; Khajavi, Mohammad S.
 CORPORATE SOURCE: Chemistry Department, Shahid Beheshti University, Tehran, 19839, Iran
 SOURCE: Journal of Chemical Research, Synopses (1998), (11), 702-703
 CODEN: JRPSDC; ISSN: 0308-2342
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Synthesis of the title compds. by cyclocondensation of anthranilic acid, formic acid (or an ortho ester) and an amine in one pot under microwave irradiation takes place in a few minutes.

RX(10) OF 11 A + X ==> J



J
YIELD 71%

RX(10) RCT A 118-92-3, X 3342-77-6

STAGE(1)

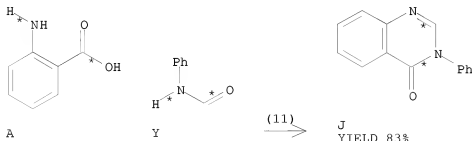
STAGE(2)

SOL 7732-18-5 Water, 64-17-5 EtOH

PRO J 16347-60-7

NTE microwave irradiation without solvent in first stage

RX(11) OF 11 A + Y ==> J



RX(11) RCT A 118-92-3, Y 103-70-8

STAGE(1)

RGT Z 127-19-5 AcNMe2

STAGE(2)

SOL 7732-18-5 Water, 64-17-5 EtOH

PRO J 16347-60-7

NTE microwave irradiation without solvent in first stage

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 122 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 129:343135 CASREACT

TITLE: Diastereoselective aziridination of alkenes using
3-acetoxyamino-2-(1-hydroxyalkyl)quinazolin-4(3H)-ones
in the presence of titanium(IV) tert-butoxide
AUTHOR(S): Atkinson, Robert S.; Ayscough, Andrew P.; Gattrell, W.
T.; Raynham, Tony M.

CORPORATE SOURCE: Dep. Chem., Univ. Leicester, LE1 7RH, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions
1: Organic and Bio-Organic Chemistry (1998), (17),
2783-2793

CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

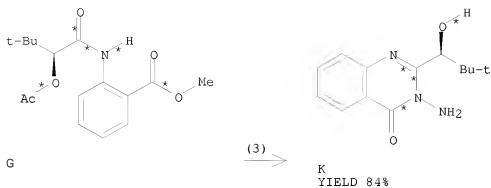
DOCUMENT TYPE: Journal

LANGUAGE: English

AB 3-Amino-2-[(S)-1-hydroxy-2,2-dimethylpropyl]quinazolin-4(3H)-one 9 (Q2NH)
was prepared in four steps from (S)-tert-leucine in 43% yield without the
need for chromatography. The corresponding 3-acetoxy-aminoquinazolinone,
prepared in dichloromethane solution by reaction of 9 with lead tetraacetate,
reacts with alkenes in the presence of titanium(IV) tert-butoxide to give
the corresponding aziridines stereoselectively. With styrene and
butadiene the corresponding aziridines were obtained completely
stereoselectively. Indene gave the expected endo-N-invertomer of
aziridine as the kinetically-formed product (86%) also completely
stereoselectively: equilibration to give a 8:1 ratio of exo:endo
N-invertomers occurs above 0°C. From an X-ray structure determination one
aziridine product, the sense of diastereoselectivity in its formation is
in agreement with the transition state model. Aziridinations of Me
acrylate and of tert-Bu acrylate give the resp. products highly
stereoselectively (dr≥20:1) and with the same sense of
diastereoselectivity as identified by an X-ray crystal structure determination
previously. Aziridinations of α-methylstyrene and Me methacrylate
are less completely diastereoselective; isoprene reacts completely
diastereoselectively at its unsubstituted double bond but with little
diastereoselectivity at its methyl-substituted double bond and the
regioselectivity of aziridination on the two double bonds is 1.4:1 resp.
by comparison to 1:4.7 in the absence of titanium(IV) tert-butoxide.

RX(3) OF 127 ...G ==> K...

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RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

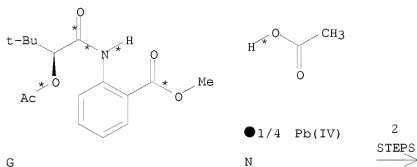
SOL 7732-18-5 Water

PRO K 182160-10-7

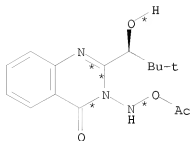
NTE STEREOSELECTIVE

RX(28) OF 127 COMPOSED OF RX(3), RX(4)

RX(28) G + N ==> O



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O

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

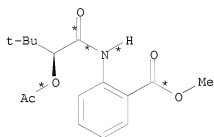
PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

RX(29) OF 127 COMPOSED OF RX(3), RX(5)

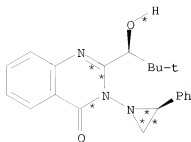
RX(29) 2 G + 2 Q ==> R + S



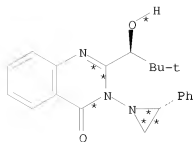
2 G

2 Q

2
STEPS
=>



R
YIELD 90% (40)



S
YIELD 90% (60)

RX(3) RCT G 21546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(5) RCT K 182160-10-7

STAGE(1)

RGT N 546-67-8 Pb(OAc)4

STAGE(2)

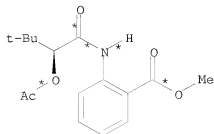
RCT Q 100-42-5

PRO R 182160-14-1, S 182267-16-9

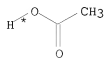
NTE STEREOSELECTIVE

RX(57) OF 127 COMPOSED OF RX(3), RX(4), RX(6)

RX(57) 2 G + 2 N + T + Q ==> R + U



2 G



● 1/4 Pb(IV)

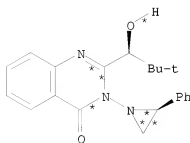
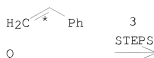
2 N



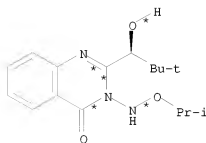
● 1/4 Ti(IV)

T

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R
YIELD 14%



U
YIELD 59%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STERESELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STERESELECTIVE

RX(6) RCT O 182160-08-3, T 546-68-9, Q 100-42-5

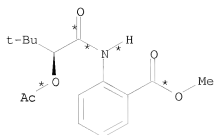
PRO R 182160-14-1, U 215546-93-3

SOL 75-09-2 CH2Cl2

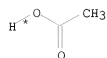
NTE STERESELECTIVE

RX(58) OF 127 COMPOSED OF RX(3), RX(4), RX(7)

RX(58) G + N + Q ==> R



G



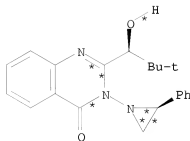
● 1/4 Pb(IV)

N



Q

3
STEPS
→



R

YIELD 65%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(7) RCT O 182160-08-3, Q 100-42-5

RGT W 3087-39-6 (t-BuO)4Ti

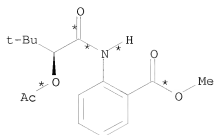
PRO R 182160-14-1

SOL 75-09-2 CH2Cl2

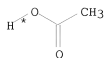
NTE STEREOSELECTIVE

RX(59) OF 127 COMPOSED OF RX(3), RX(4), RX(8)

RX(59) G + N + X ==> Y



G



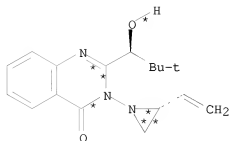
● 1/4 Pb(IV)

N



x

3
STEPS



Y
YIELD 76%

RX (3) RCT G 215546-92-2

STAGE (1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE (2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX (4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

RX(8) RCT O 182160-08-3, X 106-99-0

PRO Y 182267-17-0

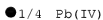
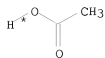
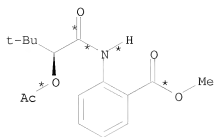
SOL 75-09-2 CH2C12

NTE STEREOSELECTIVE

RX(60) OF 127 COMPOSED OF RX(3), RX(4), RX(9)

$$RX(60) \quad G + N + X \implies Z$$

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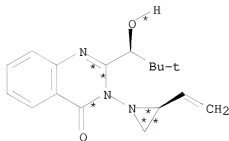


G

N

X

3
STEPS
→



Z

YIELD 85%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(9) RCT O 182160-08-3, X 106-99-0

RGT W 3087-39-6 (t-BuO)4Ti

PRO Z 182160-17-4

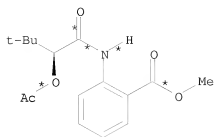
SOL 75-09-2 CH2Cl2

NTE STEREOSELECTIVE

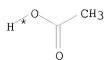
RX(61) OF 127 COMPOSED OF RX(3), RX(4), RX(10)

RX(61) G + N + AA ==> AB

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G



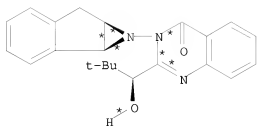
● 1/4 Pb(IV)

N



AA

3
STEPS
→



AB

YIELD 86%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

RX(10) RCT O 182160-08-3, AA 95-13-6

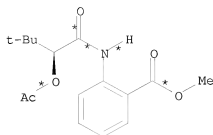
PRO AB 182267-18-1

SOL 75-09-2 CH2Cl2

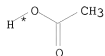
NTE STEREOSELECTIVE

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RX(62) OF 127 COMPOSED OF RX(3), RX(4), RX(11)
 RX(62) G + N + AC ==> AD



G



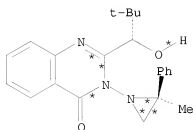
● 1/4 Pb(IV)

N



AC

3
 STEPS
 →



AD
 YIELD 77%

RX(3) RCT G 21546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

RX(11) RCT O 182160-08-3, AC 98-83-9

STAGE(1)

SOL 75-09-2 CH2Cl2

STAGE(2)

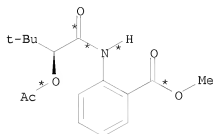
RGT AE 144-55-8 NaHCO3

SOL 7732-18-5 Water

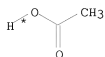
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PRO AD 215546-94-4
NTE STERESELECTIVE

RX(63) OF 127 COMPOSED OF RX(3), RX(4), RX(12)
RX(63) 2 G + 2 N + W + AC ==> AF + AD



2 G



● 1/4 Pb(IV)

2 N



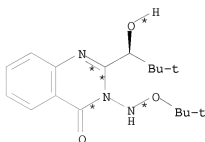
● 1/4 Ti(IV)

W

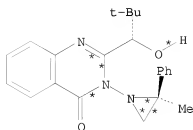


AC

3
STEPS
→



AF
YIELD 8%



AD
YIELD 44%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

RX(12) RCT O 182160-08-3, W 3087-39-6, AC 98-83-9

STAGE(1)

SOL 75-09-2 CH2Cl2

STAGE(2)

RGT AE 144-55-8 NaHCO3

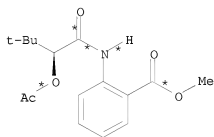
SOL 7732-18-5 Water

PRO AF 215546-95-5, AD 215546-94-4

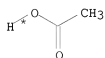
NTE STEREOSELECTIVE

RX(64) OF 127 COMPOSED OF RX(3), RX(4), RX(13)

RX(64) 4 G + 4 N + 3 AG ==> AH + AI + AJ + AK

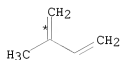


4 G

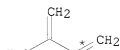


● 1/4 Pb(IV)

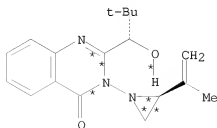
4 N

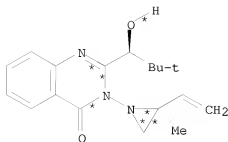


2 AG

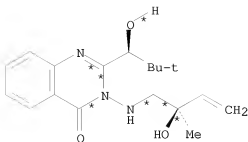


AG

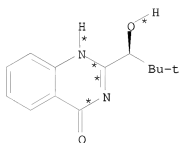
3
STEPS
→AH
YIELD 10%



AI
YIELD 48%



AJ
YIELD 10%



AK
YIELD 12%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

RX(13) RCT O 182160-08-3, AG 78-79-5

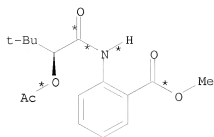
PRO AH 215546-97-7, AI 215546-96-6, AJ 215546-98-8, AK 215546-99-9

SOL 75-09-2 CH2Cl2

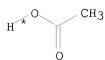
NTE STEREOSELECTIVE

RX(65) OF 127 COMPOSED OF RX(3), RX(4), RX(14)

RX(65) 2 G + 2 N + 2 AG ==> AH + AI

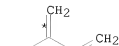


2 G

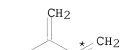


● 1/4 Pb(IV)

2 N

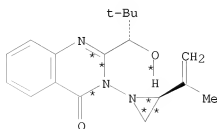


AG

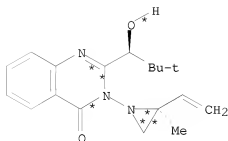


AG

3
STEPS
→



AH
YIELD 30%



AI
YIELD 30%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

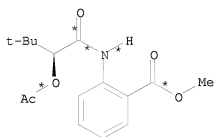
PRO K 182160-10-7

NTE STEREOSELECTIVE

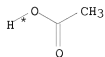
RX(4) RCT K 182160-10-7, N 546-67-8
 PRO O 182160-08-3
 SOL 865-49-6 CDC13
 NTE STEREOSELECTIVE

RX(14) RCT O 182160-08-3, AG 78-79-5
 RGT W 3087-39-6 (t-BuO) 4Ti
 PRO AH 215546-97-7, AI 215546-96-6
 SOL 75-09-2 CH2C12
 NTE STEREOSELECTIVE

RX(66) OF 127 COMPOSED OF RX(3), RX(4), RX(15)
 RX(66) 2 G + 2 N + AL + W ==> AM + AF

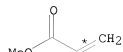


2 G



● 1/4 Pb(IV)

2 N



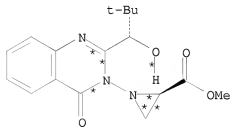
AL



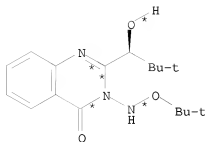
● 1/4 Ti(IV)

W

3
 STEPS
 →



AM
 YIELD 65%



AF
YIELD 25%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

RX(15) RCT O 182160-08-3, AL 96-33-3, W 3087-39-6

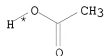
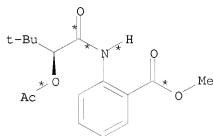
PRO AM 215547-00-5, AF 215546-95-5

SOL 75-09-2 CH2Cl2

NTE STEREOSELECTIVE

RX(67) OF 127 COMPOSED OF RX(3), RX(4), RX(16)

RX(67) G + N + AN ==> AF



● 1/4 Pb(IV)

● 1/4 Zr(IV)

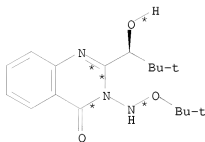
G

N

AN

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3
STEPS
→



AF
YIELD 56%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(16) RCT O 182160-08-3, AN 2081-12-1

RGT AL 96-33-3 Me acrylate

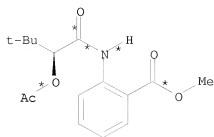
PRO AF 215546-95-5

SOL 75-09-2 CH2Cl2

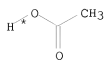
NTE STEREOSELECTIVE

RX(68) OF 127 COMPOSED OF RX(3), RX(4), RX(17)

RX(68) G + N + AO ==> U

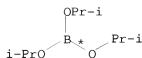


G



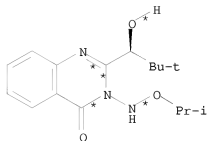
● 1/4 Pb(IV)

N



AO

3
STEPS
→



U
YIELD 75%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl3

NTE STEREOSELECTIVE

RX(17) RCT O 182160-08-3, AO 5419-55-6

RGT AL 96-33-3 Me acrylate

PRO U 215546-93-3

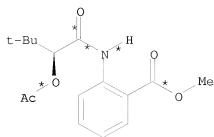
SOL 75-09-2 CH2Cl2

NTE STEREOSELECTIVE

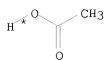
RX(69) OF 127 COMPOSED OF RX(3), RX(4), RX(18)

RX(69) 2 G + 2 N + 2 AL ==> AM + AP

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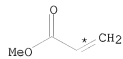


2 G



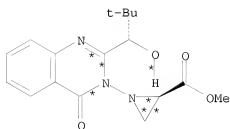
● 1/4 Pb(IV)

2 N

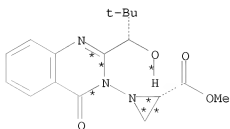


2 AL

3
STEPS
→



AM
YIELD 74% (25)



AP
YIELD 74% (75)

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

RX(18) RCT O 182160-08-3, AL 96-33-3

PRO AM 215547-00-5, AP 215547-01-6

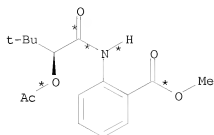
SOL 75-09-2 CH2Cl2

NTE STEREOSELECTIVE

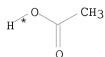
10/ 562,112

RX(70) OF 127 COMPOSED OF RX(3), RX(4), RX(22)

RX(70) 3 G + 3 N + 2 AV ==> AK + AU + AW

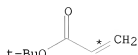


3 G



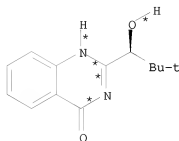
● 1/4 Pb(IV)

3 N

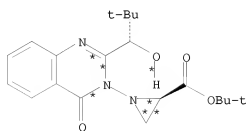


2 AV

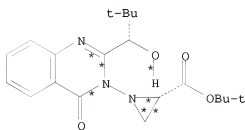
3
STEPS
→



AK
YIELD 23%



AU
YIELD 57% (48)



AW
YIELD 57% (52)

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

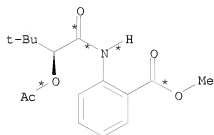
10/ 562,112

PRO K 182160-10-7
NTE STEREOSELECTIVE

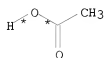
RX(4) RCT K 182160-10-7, N 546-67-8
PRO O 182160-08-3
SOL 865-49-6 CDC13
NTE STEREOSELECTIVE

RX(22) RCT O 182160-08-3, AV 1663-39-4
PRO AK 215546-99-9, AU 215547-03-8, AW 215547-02-7
SOL 75-09-2 CH2Cl2
NTE STEREOSELECTIVE

RX(71) OF 127 COMPOSED OF RX(3), RX(4), RX(23)
RX(71) 2 G + 2 N + AV + W ==> AU + AF

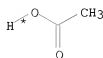


2 G



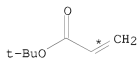
● 1/4 Pb(IV)

N



● 1/4 Pb(IV)

N



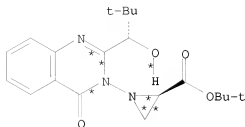
AV



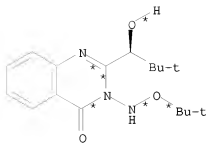
● 1/4 Ti(IV)

W

3
STEPS
=>



AU
YIELD 53%



AF
YIELD 26%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

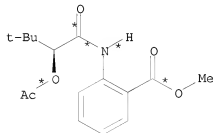
RX(23) RCT O 182160-08-3, AV 1663-39-4, W 3087-39-6

PRO AU 215547-03-8, AF 215546-95-5

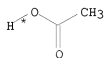
NTE STEREOSELECTIVE

RX(72) OF 127 COMPOSED OF RX(3), RX(4), RX(24)

RX(72) 2 G + 2 N + 2 AX ==> AY + AZ

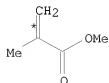


2 G



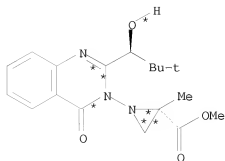
● 1/4 Pb(IV)

2 N

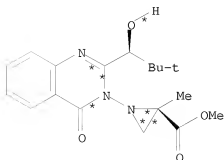


2 AX

3
STEPS
→



AY
YIELD 79% (32)



AZ
YIELD 79% (68)

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

RX(24) RCT O 182160-08-3, AX 80-62-6

PRO AY 215547-05-0, AZ 215547-04-9

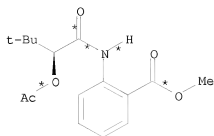
SOL 75-09-2 CH2Cl2

NTE STEREOSELECTIVE

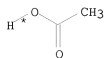
RX(73) OF 127 COMPOSED OF RX(3), RX(4), RX(25)

10/ 562,112

RX(73) 3 G + 3 N + 2 AX + W ==> AY + AZ + AF

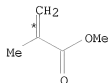


3 G



● 1/4 Pb(IV)

3 N



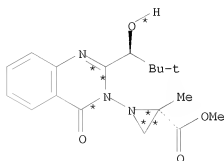
2 AX



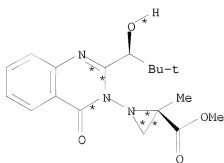
● 1/4 Ti(IV)

W

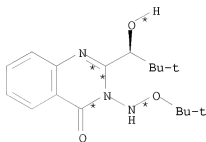
3
STEPS
→



AY
YIELD 45%(87)



AZ
YIELD 45%(13)



AF
YIELD 28%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

RX(25) RCT O 182160-08-3, AX 80-62-6, W 3087-39-6

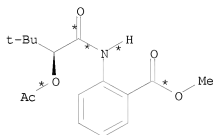
PRO AY 215547-05-0, AZ 215547-04-9, AF 215546-95-5

SOL 75-09-2 CH2Cl2

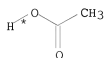
NTE STEREOSELECTIVE

RX(96) OF 127 COMPOSED OF RX(3), RX(4), RX(15), RX(19)

RX(96) 2 G + 2 N + AL + W ==> AQ

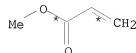


2 G



● 1/4 Pb(IV)

2 N

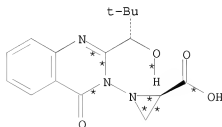


AL



● 1/4 Ti(IV)

W

4
STEPS
→AQ
YIELD 88%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7
 NTE STEREOSELECTIVE

 RX(4) RCT K 182160-10-7, N 546-67-8
 PRO O 182160-08-3
 SOL 865-49-6 CDC13
 NTE STEREOSELECTIVE

 RX(15) RCT O 182160-08-3, AL 96-33-3, W 3087-39-6
 PRO AM 215547-00-5, AF 215546-95-5
 SOL 75-09-2 CH2Cl2
 NTE STEREOSELECTIVE

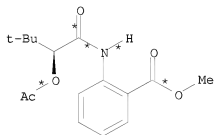
 RX(19) RCT AM 215547-00-5

 STAGE(1)
 RGT AR 1310-73-2 NaOH
 SOL 64-17-5 EtOH, 7732-18-5 Water

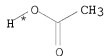
 STAGE(2)
 RGT AS 7664-93-9 H2SO4

 PRO AQ 215547-06-1
 NTE STEREOSELECTIVE

RX(97) OF 127 COMPOSED OF RX(3), RX(4), RX(18), RX(19)
 RX(97) 2 G + 2 N + 2 AL ==> AQ

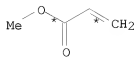


2 G

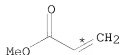


● 1/4 Pb(IV)

2 N

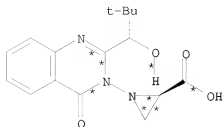


AL



AL

4
STEPS
→



AQ
YIELD 88%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

RX(18) RCT O 182160-08-3, AL 96-33-3

PRO AM 215547-00-5, AP 215547-01-6

SOL 75-09-2 CH2Cl2

NTE STEREOSELECTIVE

RX(19) RCT AM 215547-00-5

STAGE(1)

RGT AR 1310-73-2 NaOH

SOL 64-17-5 EtOH, 7732-18-5 Water

STAGE(2)

RGT AS 7664-93-9 H2SO4

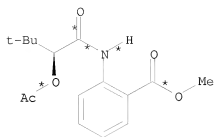
PRO AQ 215547-06-1

NTE STEREOSELECTIVE

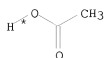
RX(98) OF 127 COMPOSED OF RX(3), RX(4), RX(18), RX(20)

RX(98) 2 G + 2 N + 2 AL ==> AT

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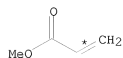


2 G

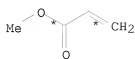


● 1/4 Pb(IV)

2 N

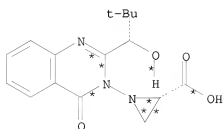


AL



AL

4
STEPS
→



AT

YIELD 88%

RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N2H4

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDC13

NTE STEREOSELECTIVE

RX(18) RCT O 182160-08-3, AL 96-33-3

PRO AM 215547-00-5, AP 215547-01-6

SOL 75-09-2 CH2Cl2

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NTE STEREOSELECTIVE

RX(20) RCT AP 215547-01-6

STAGE(1)

RGT AR 1310-73-2 NaOH

SOL 64-17-5 EtOH, 7732-18-5 Water

STAGE(2)

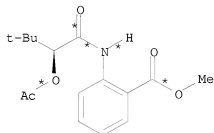
RGT AS 7664-93-9 H2SO4

PRO AT 215547-07-2

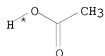
NTE STEREOSELECTIVE

RX(99) OF 127 COMPOSED OF RX(3), RX(4), RX(22), RX(21)

RX(99) 3 G + 3 N + 2 AV ==> AQ

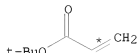


3 G

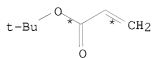


● 1/4 Pb(IV)

3 N

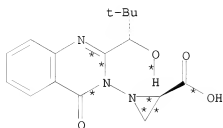


AV



AV

4
STEPS
→



AQ

YIELD 56%

RX(3) RCT G 215546-92-2

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STAGE(1)

RGT L 302-01-2 N2H4
SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7
NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8
PRO O 182160-08-3
SOL 865-49-6 CDC13
NTE STEREOSELECTIVE

RX(22) RCT O 182160-08-3, AV 1663-39-4
PRO AK 215546-99-9, AU 215547-03-8, AW 215547-02-7
SOL 75-09-2 CH2Cl2
NTE STEREOSELECTIVE

RX(21) RCT AU 215547-03-8

STAGE(1)

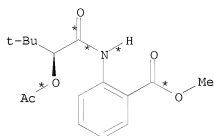
RGT AR 1310-73-2 NaOH
SOL 64-17-5 EtOH, 7732-18-5 Water

STAGE(2)

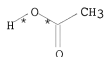
RGT AS 7664-93-9 H2SO4

PRO AQ 215547-06-1
NTE STEREOSELECTIVE

RX(100) OF 127 COMPOSED OF RX(3), RX(4), RX(23), RX(21)
RX(100) 2 G + 2 N + AV + W ==> AQ

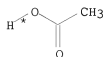


2 G



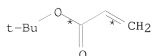
● 1/4 Pb(IV)

N

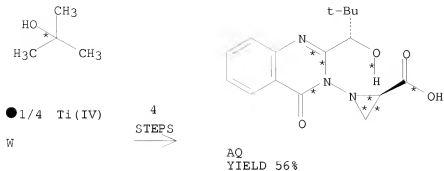


● 1/4 Pb(IV)

N



AV



RX(3) RCT G 215546-92-2

STAGE(1)

RGT L 302-01-2 N₂H₄

SOL 64-17-5 EtOH

STAGE(2)

SOL 7732-18-5 Water

PRO K 182160-10-7

NTE STEREOSELECTIVE

RX(4) RCT K 182160-10-7, N 546-67-8

PRO O 182160-08-3

SOL 865-49-6 CDCl₃

NTE STEREOSELECTIVE

RX(23) RCT O 182160-08-3, AV 1663-39-4, W 3087-39-6

PRO AU 215547-03-8, AF 215546-95-5

NTE STEREOSELECTIVE

RX(21) RCT AU 215547-03-8

STAGE(1)

RGT AR 1310-73-2 NaOH

SOL 64-17-5 EtOH, 7732-18-5 Water

STAGE(2)

RGT AS 7664-93-9 H₂SO₄

PRO AQ 215547-06-1

NTE STEREOSELECTIVE

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 123 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 128:257597 CASREACT

TITLE: Total Synthesis of the Quinazoline Alkaloids

(-)-Fumiquinazoline G and (-)-Fiscalin B

AUTHOR(S): Wang, Haishan; Ganesan, A.

CORPORATE SOURCE:

Institute of Molecular and Cell Biology, National
University of Singapore, Singapore, 117609, Singapore
Journal of Organic Chemistry (1998), 63(8), 2432-2433
CODEN: JOCEAH; ISSN: 0022-3263

SOURCE:

American Chemical Society

PUBLISHER:

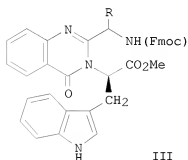
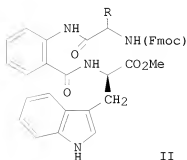
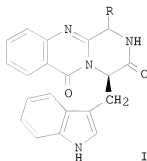
DOCUMENT TYPE:

Journal

LANGUAGE:

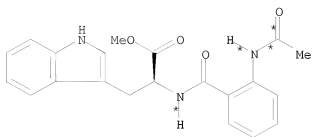
English

GI



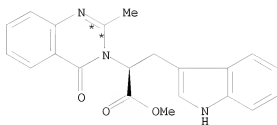
AB (-)-Fumiquinazoline G (I; R = β -Me) and (-)-fiscalin B (I; R = α -CHMe₂) were synthesized in four and five steps resp. from D-tryptophan Me ester. The key transformation involved dehydrative cyclization of linear tripeptides II (Fmoc = 9-fluorenylmethoxycarbonyl, R = β -Me, α -CHMe₂, resp.) to quinazolin-4-ones III. The methodol. is also applicable to the synthesis of quinazolinones with sterically bulky 2,3-substitution.

RX(3) OF 20 I ==> J



I

(3) →

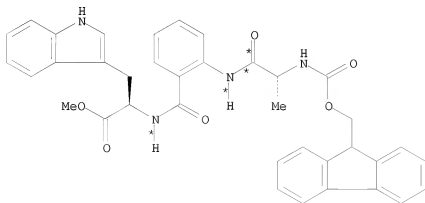


J

YIELD 99%

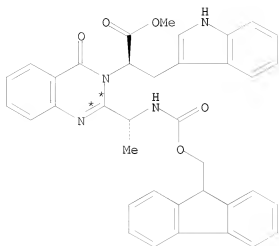
RX(3) RCT I 205042-92-8
 RGT K 603-35-0 PPh3, L 7553-56-2 I2, M 7087-68-5 EtN(Pr-i)2
 PRO J 205042-90-6
 SOL 75-09-2 CH2Cl2

RX(6) OF 20 ...S ==> A...



S

(6) →

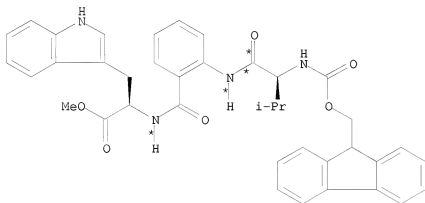


A

YIELD 65%

RX(6) RCT S 205042-95-1
 RGT K 603-35-0 PPh3, L 7553-56-2 I2, M 7087-68-5 EtN(Pr-i)2
 PRO A 205042-96-2
 SOL 75-09-2 CH2Cl2
 NTE key step

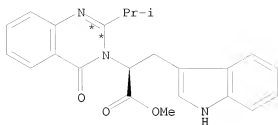
RX(8) OF 20 ...W ==> X



W

(8) →

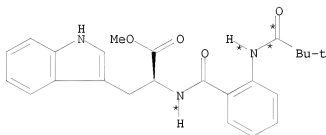
10/ 562,112



AB
YIELD 88%

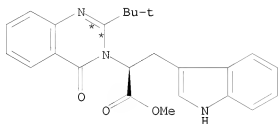
RX(10) RCT AA 205043-03-4
RGT K 603-35-0 PPh3, L 7553-56-2 I2, M 7087-68-5 EtN(Pr-i)2
PRO AB 205043-02-3
SOL 75-09-2 CH2Cl2

RX(11) OF 20 AC ==> AD



AC

(11)
→



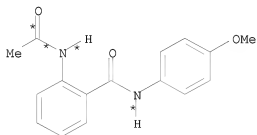
AD
YIELD 17%

RX(11) RCT AC 205043-06-7
RGT K 603-35-0 PPh3, L 7553-56-2 I2, M 7087-68-5 EtN(Pr-i)2
PRO AD 205043-04-5
SOL 75-09-2 CH2Cl2

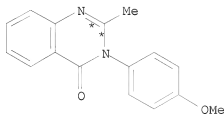
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 124 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 128:127982 CASREACT
 TITLE: An improved synthesis of 2,3-disubstituted
 4(3H)-quinazolinones from 2-acylamino-N-arylbenzamides
 AUTHOR(S): Acharya, Debi Prasad; Chattopadhyay, Subhagata
 CORPORATE SOURCE: Department of Chemistry, Jadavpur University,
 Calcutta, 700 032, India
 SOURCE: Indian Journal of Heterocyclic Chemistry (1997), 7(2),
 101-104
 CODEN: IJCHEI; ISSN: 0971-1627
 PUBLISHER: Lucknow University, Dep. of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 2-Acylamino-N-arylbenzamides on refluxing with TsOH in benzene or MeCN
 solution undergo smooth cyclodehydration to 2,3-disubstituted
 4(3H)-quinazolinones. A convenient procedure for converting isatoic
 anhydride to 2-amino-N-aryl(alkyl)benzamides is also reported.

RX(10) OF 18 V ==> W



V



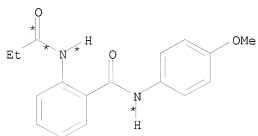
W
 YIELD 88%

RX(10) RCT V 59525-22-3
 RGT X 104-15-4 TsOH
 PRO W 30507-16-5

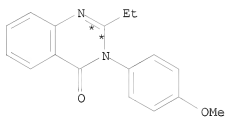
10/ 562,112

SOL 71-43-2 Benzene

RX(11) OF 18 Z ==> AA



Z

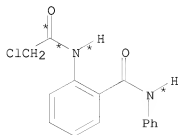


AA

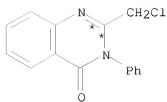
YIELD 71%

RX(11) RCT Z 25628-95-9
RGT X 104-15-4 TsOH
PRO AA 50498-62-9
SOL 71-43-2 Benzene

RX(12) OF 18 AB ==> AC



AB

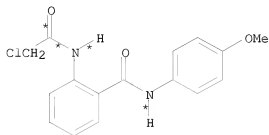


AC
YIELD 68%

10/ 562,112

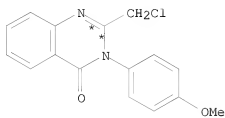
RX(12) RCT AB 18871-29-9
 RGT X 104-15-4 TsOH
 PRO AC 22312-77-2
 SOL 71-43-2 Benzene

RX(13) OF 18 AD ==> AE



AD

(13)



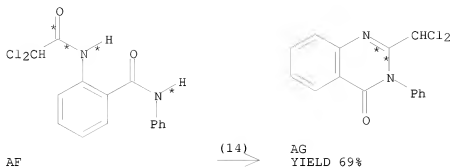
AE

YIELD 79%

RX(13) RCT AD 22312-68-1
 RGT X 104-15-4 TsOH
 PRO AE 22312-82-9
 SOL 71-43-2 Benzene

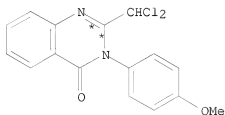
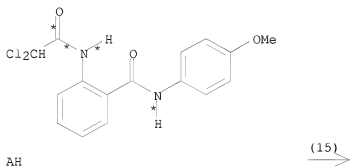
RX(14) OF 18 AF ==> AG

10/ 562,112



RX(14) RCT AF 202137-04-0
RGT X 104-15-4 TsOH
PRO AG 202137-02-8
SOL 71-43-2 Benzene

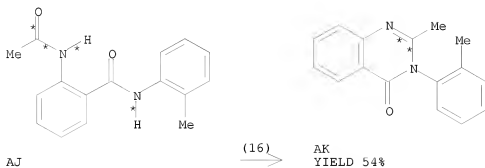
RX(15) OF 18 AH ==> AI



AI
YIELD 74%

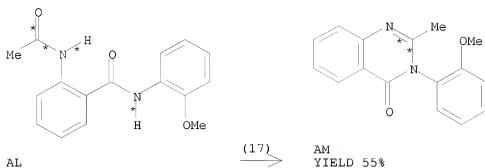
RX(15) RCT AH 202137-05-1
RGT X 104-15-4 TsOH
PRO AI 33227-62-2
SOL 71-43-2 Benzene

RX(16) OF 18 AJ ==> AK



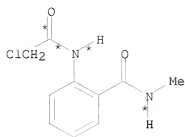
RX(16) RCT AJ 70180-39-1
 RGT X 104-15-4 TsOH
 PRO AK 72-44-6
 SOL 71-43-2 Benzene

RX(17) OF 18 AL ==> AM

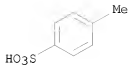


RX(17) RCT AL 92966-82-0
 RGT X 104-15-4 TsOH
 PRO AM 4260-28-0
 SOL 71-43-2 Benzene

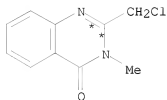
RX(18) OF 18 AN ==> AO



AN



AO: CM 1
YIELD 40%

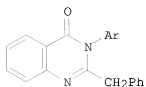


AO: CM 2
YIELD 40%

RX(18) RCT AN 53824-91-2
RGT X 104-15-4 TsOH
PRO AO 202137-03-9
SOL 71-43-2 Benzene

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

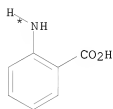
L3 ANSWER 125 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 128:102054 CASREACT
TITLE: Synthesis of some new quinazolin-4(3H)-ones as possible antimicrobial agents
AUTHOR(S): Mishra, Pradeep; Jain, Sanmati K.; Jain, Sandeep
CORPORATE SOURCE: Dep. Pharmaceutical Sci., Dr. Harisingh Gour Vishwavidyalaya, Sagar, 470 003, India
SOURCE: Journal of the Indian Chemical Society (1997), 74(10), 816-817
CODEN: JICSAH; ISSN: 0019-4522
PUBLISHER: Indian Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



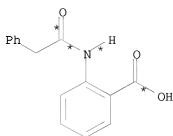
I

AB Reaction of anthranilic acid with phenacetyl chloride gave o-(phenacetyl amino)benzoic acid which on cyclization in presence of acetic anhydride gave 2-phenylmethyl-3,1-benzoxazin-4-one. Condensation of the latter with aromatic amines gave title compds. I (Ar = 3-C₆H₄OH, Ph, 2-C₆H₄CO₂H, 4-C₆H₄Br, 2-C₆H₄NO₂, 4-C₆H₄CO₂H, 3-C₆H₄NO₂, 4-C₆H₄NO₂). Bactericidal activity of some of the compds. prepared is discussed.

RX(2) OF 3 ...A + C ==> D

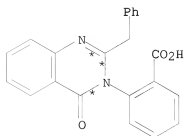


A



C

(2) →



D

YIELD 48%

RX(2) RCT A 118-92-3, C 28565-98-2
 RGT E 64-19-7 AcOH, F 108-24-7 Ac2O
 PRO D 201293-02-9
 NTE 4-6 H

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

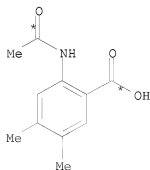
L3 ANSWER 126 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 127:205586 CASREACT
 TITLE: Preparation of 5,6-dihydro-3H-pyrimidin-4-one derivatives.
 INVENTOR(S): Bhattacharya, Apurba; Allen, Diane E.
 PATENT ASSIGNEE(S): Hoechst Celanese Corp., USA
 SOURCE: PCT Int. Appl., 29 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9728132	A1	19970807	WO 1997-US1860	19970130
W: CN, JP				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5763608	A	19980609	US 1996-595885	19960205
IN 182629	A1	19990522	IN 1997-CA107	19970120
PRIORITY APPLN. INFO.:			US 1996-595885	19960205

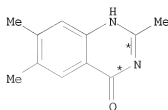
OTHER SOURCE(S): MARPAT 127:205586

AB 5,6-Dihydro-3H-pyrimidin-4-one derivs. were prepared by (a) dehydrating N-acyl β -amino acid derivs. in the presence of a dehydrating agent and an organic solvent to form oxazones; (b) adding a carboxylic acid and a primary amine salt of a carboxylic acid to said oxazones to form a mixture; (c) distilling azeotropically said mixture to remove the dehydrating agent and organic solvent; and (d) heating the product of step (c). Thus, 2-acetylamino-4,5-dimethylbenzoic acid (preparation given) was refluxed 3 h with Ac₂O and heptane; NH₄OAc was added followed by distillation of heptane, addition of AcOH, continued distillation, and reflux for 12 h to give 80% 2,6,7-trimethyl-4(3H)-quinazolinone.

RX(1) OF 1 A ==> B



A



B
YIELD 80%

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RX(1) RCT A 15089-80-2

STAGE(1)

RGT C 108-24-7 Ac2O

SOL 142-82-5 Heptane

STAGE(2)

RGT D 631-61-8 NH4OAc, E 64-19-7 AcOH

PRO B 119063-78-4

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 127 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 127:190527 CASREACT
TITLE: Three-step process for preparing anthranilic acids
from anilines
INVENTOR(S): Bhattacharya, Apurba; Allen, Diane E.
PATENT ASSIGNEE(S): Hoechst Celanese Corp., USA
SOURCE: PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 9728118	A1	19970807	WO 1997-US1862	19970130

W: CN, JP

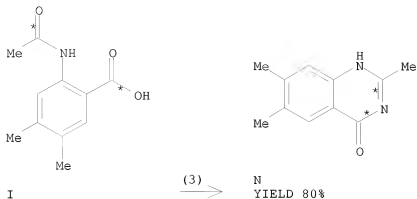
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

PRIORITY APPLN. INFO.: US 1996-596536 19960205

OTHER SOURCE(S): MARPAT 127:190527

AB Anthranilic acids, useful as cyclocondensation intermediates in the preparation of 4-quinazolinones, are prepared in high yield and selectivity by: (a) acylating an aniline with an acylation agent (e.g., Ac2O) to form the corresponding amide; (b) subjecting the acetylated intermediate to halogenation in the presence of an oxidizing agent (e.g., H2O2) to form an ortho-halogenated aniline amide; and (c) subjecting the ortho-halogenated aniline amide to carbonylation to form the anthranilic acid. Thus, 3,4-dimethylaniline was acylated with Ac2O, brominated with Br2 and H2O2, and carbonylated in the presence of CO, PPh3, and (PPh3)2PdCl2, producing 2-(acetylamino)-4,5-dimethylbenzoic acid.

RX(3) OF 6 ...I ==> N



RX(3) RCT I 15089-80-2

STAGE(1)

SOL 142-82-5 Heptane, 108-24-7 Ac2O

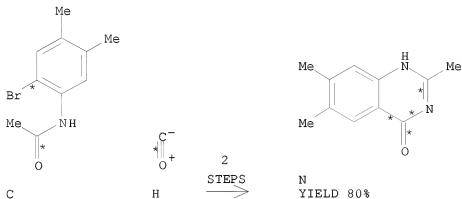
STAGE(2)

RGT O 631-61-8 NH4OAc

PRO N 119063-78-4

RX(5) OF 6 COMPOSED OF RX(2), RX(3)

RX(5) C + H ==> N



RX(2) RCT C 22364-28-9, H 630-08-0

RGT J 102-82-9 Bu3N

PRO I 15089-80-2

CAT 7439-95-4 Mg, 13965-03-2 PdCl2(PPh3)2

SOL 108-88-3 PhMe

RX(3) RCT I 15089-80-2

STAGE(1)

SOL 142-82-5 Heptane, 108-24-7 Ac2O

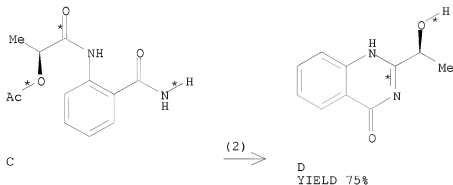
STAGE(2)
RGT O 631-61-8 NH4OAc

PRO N 119063-78-4

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 128 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 127:162006 CASREACT
 TITLE: Comments on the asymmetric synthesis of chrysogine
 AUTHOR(S): Bergman, Jan
 CORPORATE SOURCE: Department Organic Chemistry, Institute Biosciences
 Novum, Huddinge, S-141 57, Swed.
 SOURCE: Journal of Chemical Research, Synopses (1997), (6),
 224
 CODEN: JRPSCD; ISSN: 0308-2342
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The absolute configuration of the mold metabolite chrysogine,
 (S)-(-)-2-(1-hydroxyethyl)quinazolin-4(3H)-one, was first determined by asym.
 synthesis in 1990 and not in 1996 as recently claimed.

RX(2) OF 3 ...C ==> D



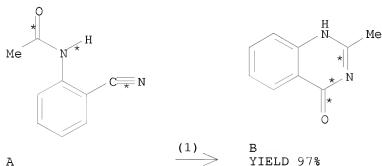
RX(2) RCT C 129768-43-0
 PRO D 42599-89-3

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 129 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 126:330589 CASREACT
 TITLE: Synthesis of quinazolin-4(3H)-ones from
 o-amidobenzonitriles using urea-hydrogen peroxide
 AUTHOR(S): Bandgar, B. P.

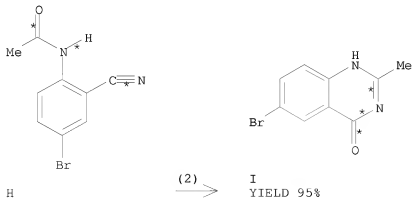
CORPORATE SOURCE: Department of Chemistry, Post Graduate and Research Centre, R. B. N. B. College, Shrirampur, 413709, India
 SOURCE: Synthetic Communications (1997), 27(12), 2065-2068
 CODEN: SYNCAV; ISSN: 0039-7911
 PUBLISHER: Dekker
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Synthesis of quinazolin-4(3H)-ones from o-amidobenzonitriles has been carried out by using urea-hydrogen peroxide as a mild, stable and non-hazardous reagent.

RX(1) OF 7 A ==> B



RX(1) RCT A 25116-00-1
 RGT C 57-13-6 Urea, D 7722-84-1 H2O2
 PRO B 1769-24-0
 CAT 584-08-7 K2CO3
 SOL 7732-18-5 Water, 67-64-1 Me2CO

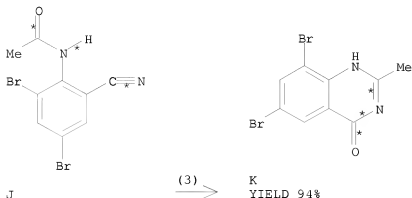
RX(2) OF 7 H ==> I



RX(2) RCT H 189634-99-9
 RGT C 57-13-6 Urea, D 7722-84-1 H2O2
 PRO I 5426-59-5
 CAT 584-08-7 K2CO3

SOL 7732-18-5 Water, 67-64-1 Me2CO

RX(3) OF 7 J ==> K



RX(3) RCT J 189635-00-5
 RGT C 57-13-6 Urea, D 7722-84-1 H2O2
 PRO K 82326-77-0
 CAT 584-08-7 K2CO3
 SOL 7732-18-5 Water, 67-64-1 Me2CO

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

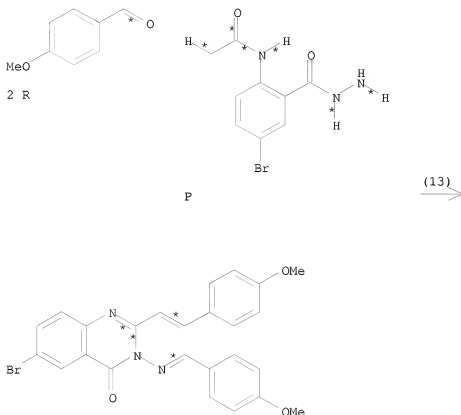
L3 ANSWER 130 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 125:10738 CASREACT
 TITLE: Chemoselectivity of
 6-bromo-2-methyl-3,1-benzoxazin-4-one towards amines,
 Schiff bases, and azines
 AUTHOR(S): Derbala, H. A.
 CORPORATE SOURCE: Chem. Dep., Ain Shams Univ., Cairo, Egypt
 SOURCE: Monatshefte fuer Chemie (1996), 127(1), 103-10
 CODEN: MOCMB7; ISSN: 0026-9247
 PUBLISHER: Springer
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 6-Bromo-2-methyl-3,1-benzoxazin-4-one (1) undergoes an unusual cleavage at position 4 when it is allowed to react with o-phenylenediamine or anthranilic acid in dry benzene to give the corresponding compds. I,II,III,IV, resp. The reaction of 1 with Schiff bases and azines results in the formation of the compds. V [R,R' given: H,H;p-MeO,H;H,p-Cl;3,4-(MeO)2,H] and VI(R2-H,p-MeO), resp. The reaction involves a cleavage of the Schiff base or the azine into its amine and

arylidene moieties which are smoothly incorporated into 1 via nucleophilic attack of the amine at position 4 and condensation of the aldehyde with a reactive Me group, at position 2 resp. No displacement of the arylidene segment was observed

RX(13) OF 14 ...2 R + P ==> S



S
YIELD 63%

RX(13) RCT R 123-11-5, P 71822-95-2
RGT K 64-19-7 AcOH, L 127-09-3 AcONa
PRO S 175877-95-9
NTE 6 H

L3 ANSWER 131 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 122:81279 CASREACT
TITLE: Facile synthesis of
2-alkyl-3-aryl-4(3H)-quinazolinones
AUTHOR(S): Ramana, D. V.; Kantharaj, E.
CORPORATE SOURCE: Department Chemistry, Indian Institute Technology,
Madras, 600 036, India
SOURCE: Indian Journal of Heterocyclic Chemistry (1994), 3(4),

215-18

CODEN: IJCHEI; ISSN: 0971-1627

DOCUMENT TYPE:

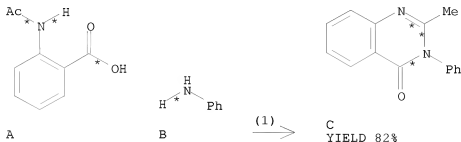
Journal

LANGUAGE:

English

AB The synthesis of 2-alkyl-3-aryl-4(3H)-quinazolinones was achieved in good yields under mild conditions by reaction of N-acylantranilic acids with tosyl chloride in pyridine at room temperature followed by the addition of amine.

RX(1) OF 4 A + B ==> C



RX(1) RCT A 89-52-1

STAGE(1)

RGT D 98-59-9 TsCl

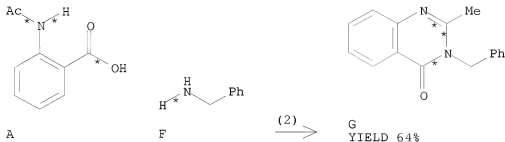
SOL 110-86-1 Pyridine

STAGE(2)

RCT B 62-53-3

PRO C 2385-23-1

RX(2) OF 4 A + F ==> G



RX(2) RCT A 89-52-1

STAGE(1)

RGT D 98-59-9 TsCl

SOL 110-86-1 Pyridine

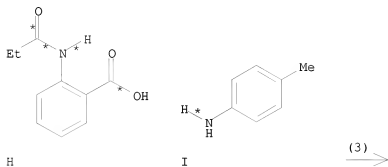
STAGE(2)

RCT F 100-46-9

10/ 562,112

PRO G 4260-34-8

RX(3) OF 4 H + I ==> J



J
YIELD 70%

RX(3) RCT H 19165-26-5

STAGE(1)

RGT D 98-59-9 TsCl

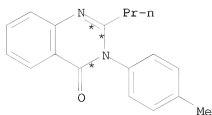
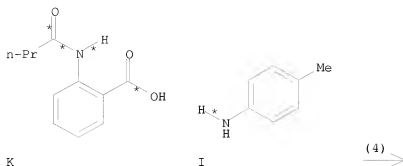
SOL 110-86-1 Pyridine

STAGE(2)

RCT I 106-49-0

PRO J 50498-61-8

RX(4) OF 4 K + I ==> L



L
YIELD 78%

RX(4) RCT K 6328-94-5

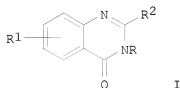
STAGE(1)
RGT D 98-59-9 TsCl
SOL 110-86-1 Pyridine

STAGE(2)
RCT I 106-49-0

PRO L 84312-85-6

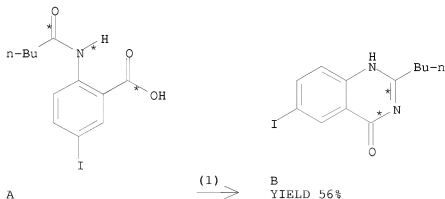
L3 ANSWER 132 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 121:255825 CASREACT
 TITLE: Process for the preparation of 2-alkyl-3,5,6,7- or 8-substituted-4-(3H)-quinazolinones via heterocyclization of N-acylanthranilic acids with ethyl chloroformate and ammonia/amine
 INVENTOR(S): Mohan, Arthur G.; D, Antuono, Joseph III.
 PATENT ASSIGNEE(S): American Cyanamid Company, USA
 SOURCE: U.S., 6 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5342944	A	19940830	US 1993-92850	19930719
PRIORITY APPLN. INFO.:			US 1993-92850	19930719
OTHER SOURCE(S):		MARPAT 121:255825		
GI				



AB A novel process for producing 2-alkyl-3,5,6,7 or 8-substituted-4(3H)-quinazolinones of the formula I (R is selected from H, straight or branched alkyl of 1 to 9 carbon atoms, Ph, substituted Ph, etc.; R1 is a straight or branched alkyl of 1 to 9 carbon atoms, optionally substituted with a substituent selected from H, straight chain alkyl of 1 to 4 carbon atoms, Ph, substituted Ph, etc.; R2 is a straight chain alkyl of 1 to 6 carbon atoms) consists of reacting the appropriate N-acyl substituted aminobenzoic acids with Et chloroformate followed by further reaction with ammonia or a primary amine. Thus, e.g., to N-valeryl-5-iodoanthranilic acid in DMF is added Et3N and Et chloroformate; the reaction mixture is heated to 2 h until the evolution of carbon dioxide ceases, and then concentrated ammonium hydroxide is added; workup afforded 56.7% 2-Butyl-6-iodo-4-(3H)-quinazolinone.

RX(1) OF 1 A ==> B



RX(1) RCT A 158591-92-5

STAGE(1)

RGT C 121-44-8 Et3N, D 541-41-3 ClCO2Et
SOL 68-12-2 DMF

STAGE(2)

RGT E 1336-21-6 NH4OH

SOL 7732-18-5 Water

PRO B 143945-48-6

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 133 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 121:35482 CASREACT

TITLE: Synthesis and reactions of substituted benzoxazinones bearing a bulky group at position 2

AUTHOR(S): Soliman, F. M. A.; Souka, L. M.; Eslam, I. E.; Dawood, N. T. A.

CORPORATE SOURCE: Fac. Sci., Al-Azhar Univ., Cairo, Egypt

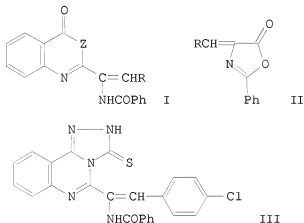
SOURCE: Revue Roumaine de Chimie (1992), 37(10), 1153-8

CODEN: RRCHAX; ISSN: 0035-3930

DOCUMENT TYPE: Journal

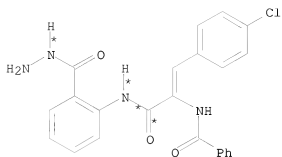
LANGUAGE: English

GI

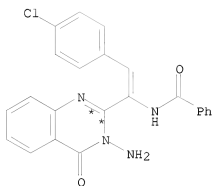


AB 2-Substituted 3,1-benzoxazin-4-ones I (Z = O, R = Ph or substituted phenyl) were prepared by reaction of oxazolones II with anthranilic acid. Reactions of I with amines and sodium azides were carried out. Thus, treatment of I (Z = O, R = p-ClC6H4) with H2NOH.HCl or semicarbazide gave quinazolinone I (Z = N, R = p-ClC6H4) and triazole III, resp.

RX(18) OF 52 ...AC ==> AH



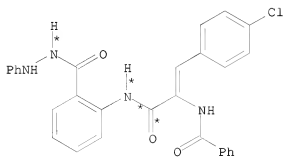
AC

(18) \longrightarrow 

AH

RX(18) RCT AC 132994-54-8
 PRO AH 132994-59-3

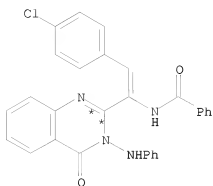
RX(19) OF 52 ...AE ==> AI



AE

(19) \longrightarrow

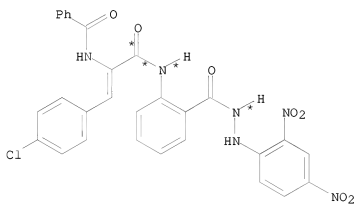
10/ 562,112



AI

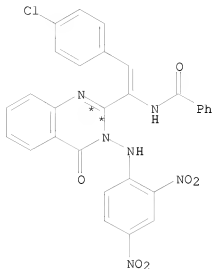
RX(19) RCT AE 132994-55-9
 PRO AI 142075-10-3

RX(20) OF 52 ...AG ==> AJ



AG

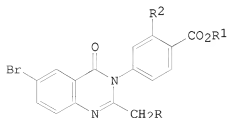
(20)



AJ

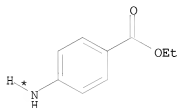
RX(20) RCT AG 141264-77-9
PRO AJ 142075-11-4

L3 ANSWER 134 OF 258 CASREACT COPYRIGHT 2009 ACS on SIN
ACCESSION NUMBER: 120:323466 CASREACT
TITLE: Synthesis and biological activities of
6-bromo-2,3-disubstituted-4-(3H)-quinazolinones
AUTHOR(S): Abdel-Alim, Abdel-Alim M.; El-Shorbegi, Abdel-Nasser
A.; El-Shareif, Hosny A. H.; El-Gendy, Mahmoud A.;
Amin, Monir A.
CORPORATE SOURCE: Fac. Pharm., Assiut Univ., Cairo, Egypt
SOURCE: Indian Journal of Chemistry, Section B: Organic
Chemistry Including Medicinal Chemistry (1994),
33B(3), 260-5
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

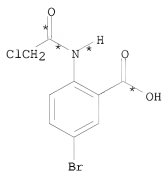


AB The title compds., 6-bromo-2, 3-disubstituted-4(3H)-quinazolinones (I) have been synthesized for evaluation as potential sedative-hypnotic, anti-convulsant and anti-inflammatory agents. Compound I (R = PhCH₂S, R₁ = Et, R₂ = H) has been synthesized by condensing 6-bromo-2-chloromethyl-3-(p-ethoxycarbonylphenyl)-4(3H)-quinazolinone with benzyl mercaptan in the presence of potassium carbonate. Compds. I (R = CH₂SCCH₂CO₂H, CH₂SCCH₂CH₂CO₂H, CH₂SCCHMeCO₂H) (II) are obtained by the condensation of I (R = Cl) with the appropriate thioacid. Superior sedative-hypnotic and anti-convulsant effects are achieved by II (R₁ = Me, Et: R₂ = H) (III). On the other hand, II (R₂ = OH) reveal better results as anti-inflammatory agents than that for III. Most of the tested compds. have been found to be, at least, two times as potent as aspirin in anti-inflammatory tests.

RX(1) OF 1 A + B ==> C



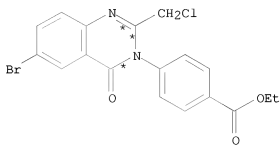
A



B



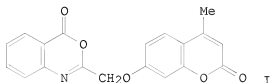
(1) → C
YIELD 72%



RX(1) RCT A 94-09-7, B 155104-20-4
 RGT D 7719-12-2 PC13
 PRO C 155104-08-8
 SOL 1330-20-7 Xylene

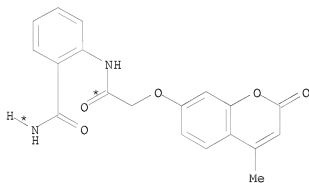
L3 ANSWER 135 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 120:323426 CASREACT
TITLE: Synthesis and reactions of
 2-[[[4-methyl-2-oxo-2H-[1]benzopyran-7-yl]oxy]methyl]-

4H-3,1-benzoxazin-4-one
 AUTHOR(S): Soliman, A. Y.; El-Assy, N. B.; El-Shahed, F.;
 El-Kady, M.; El-Deen, I. M.
 CORPORATE SOURCE: Fac. Sci, Ain Shams Univ., Egypt
 SOURCE: Revue Roumaine de Chimie (1993), 38(1), 83-9
 CODEN: RRCHAX; ISSN: 0035-3930
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



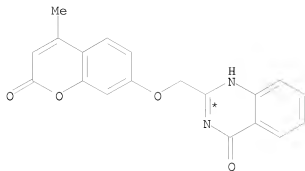
AB The relative reactivities of the α -pyrone and oxazinone rings in I
 (title compound) with nucleophiles (Friedel-Crafts arylation, aminolysis,
 and hydrazinolysis) and electrophiles (aromatic aldehydes) are compared.

RX(15) OF 67 ...AC ==> AD



AC

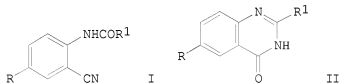
(15) \longrightarrow



AD
YIELD 65%

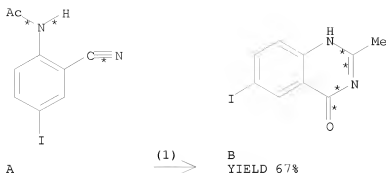
RX(15) RCT AC 128649-83-2
RGT AE 108-24-7 Ac2O
PRO AD 128649-84-3

L3 ANSWER 136 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 120:217532 CASREACT
TITLE: A facile preparation of quinazolin-4(3H)-ones from
o-amido benzonitriles using sodium perborate
AUTHOR(S): Baudoin, Bernard; Ribeill, Yves; Vicker, Nigel
CORPORATE SOURCE: Dagenham Res. Cent., Rhone-Poulenc Rorer Ltd.,
Dagenham/Essex, RM10 7XS, UK
SOURCE: Synthetic Communications (1993), 23(20), 2833-7
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



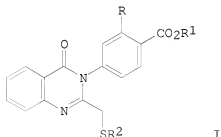
AB The oxidation of o-amidobenzonitriles I (R = iodo, R1 = Me, ethylcyclohexyl; R = H, R1 = Ph; R = 3,4,5-trimethoxystyryl, R1 = Me2N, ethylcyclohexyl) using sodium perborate followed by cyclization afforded quinazolin-4(3H)-ones II in a one-pot reaction under mild, non-hazardous conditions.

RX(1) OF 1 A ==> B



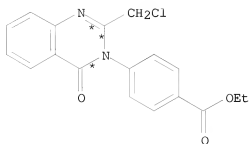
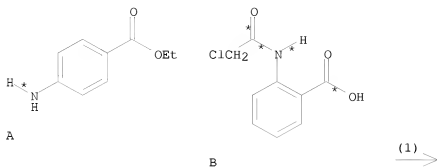
RX(1) RCT A 153861-34-8
 RGT C 7632-04-4 NaBO3
 PRO B 90347-75-4
 SOL 7732-18-5 Water, 123-91-1 Dioxane

L3 ANSWER 137 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 120:217521 CASREACT
 TITLE: Quinazolinone derivatives of biological interest. V.
 Novel 4(3H)-quinazolinones with sedative-hypnotic,
 anticonvulsant and antiinflammatory activities
 AUTHOR(S): Abdel-Alim, Abdel-Alim M.; El-Shorbagi, Nasser A.;
 El-Gendy, Mahmoud A.; El-Shareif, Hosny A. H.
 CORPORATE SOURCE: Pharm. Chem. Dep., Assiut Univ., Assiut, Egypt
 SOURCE: Collection of Czechoslovak Chemical Communications
 (1993), 58(8), 1963-8
 CODEN: CCCCAK; ISSN: 0010-0765
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The title compds., I (R = H, HO; R1 = alkyl; R2 = Ph, benzyl, carboxyalkyl, etc.) and derivs. thereof were prepared. Their pharmacol. activity data for I as sedatives, hypnotics, anticonvulsants and inflammation inhibitors, analgesics, or antipyretics were not reported.

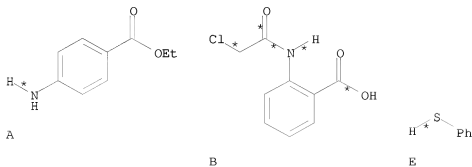
RX(1) OF 17 A + B ==> C...



YIELD 76%

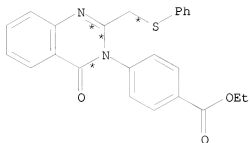
RX(1) RCT A 94-09-7, B 14422-49-2
 RGT D 7719-12-2 PC13
 PRO C 76535-04-1

RX(10) OF 17 COMPOSED OF RX(1), RX(2)
 RX(10) A + B + E ==> F



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2
STEPS
→

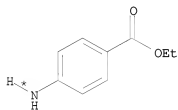


F
YIELD 79%

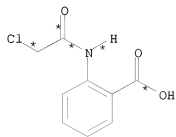
RX(1) RCT A 94-09-7, B 14422-49-2
RGT D 7719-12-2 PC13
PRO C 76535-04-1

RX(2) RCT E 108-98-5, C 76535-04-1
PRO F 153705-92-1

RX(11) OF 17 COMPOSED OF RX(1), RX(3)
RX(11) A + B + G ==> H



A



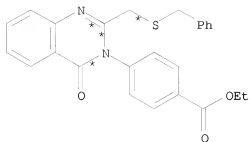
B



G

2
STEPS
→

10/ 562,112

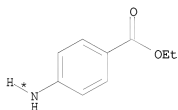


H
YIELD 81%

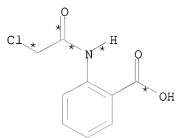
RX(1) RCT A 94-09-7, B 14422-49-2
RGT D 7719-12-2 PC13
PRO C 76535-04-1

RX(3) RCT G 100-53-8, C 76535-04-1
PRO H 153705-94-3

RX(12) OF 17 COMPOSED OF RX(1), RX(4)
RX(12) A + B + I ==> J



A

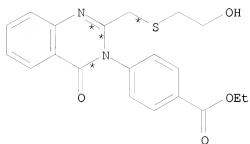


B



I

2
STEPS
=>

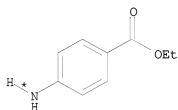


J
YIELD 75%

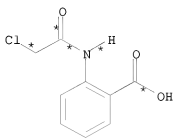
RX(1) RCT A 94-09-7, B 14422-49-2
RGT D 7719-12-2 PC13
PRO C 76535-04-1

RX(4) RCT I 60-24-2, C 76535-04-1
PRO J 153705-98-7

RX(13) OF 17 COMPOSED OF RX(1), RX(5)
RX(13) A + B + K ==> L



A



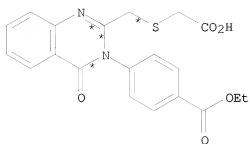
B



K

2
STEPS
=>

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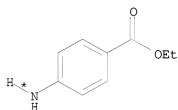


L
YIELD 78%

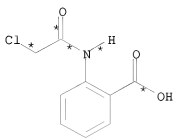
RX(1) RCT A 94-09-7, B 14422-49-2
RGT D 7719-12-2 PC13
PRO C 76535-04-1

RX(5) RCT K 68-11-1, C 76535-04-1
PRO L 137731-84-1

RX(14) OF 17 COMPOSED OF RX(1), RX(6)
RX(14) A + B + M ==> N



A



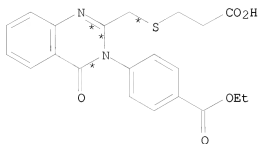
B



M

2
STEPS
=>

10/ 562,112

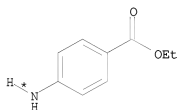


N
YIELD 81%

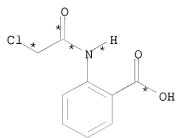
RX(1) RCT A 94-09-7, B 14422-49-2
RGT D 7719-12-2 PC13
PRO C 76535-04-1

RX(6) RCT M 107-96-0, C 76535-04-1
PRO N 137731-85-2

RX(15) OF 17 COMPOSED OF RX(1), RX(7)
RX(15) A + B + O ==> P



A

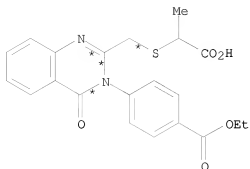


B



O

2
STEPS
=>

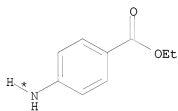


P
YIELD 69%

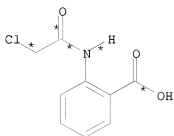
RX(1) RCT A 94-09-7, B 14422-49-2
RGT D 7719-12-2 PC13
PRO C 76535-04-1

RX(7) RCT O 79-42-5, C 76535-04-1
PRO P 137731-86-3

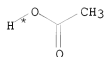
RX(16) OF 17 COMPOSED OF RX(1), RX(8)
RX(16) A + B + Q ==> R



A



B

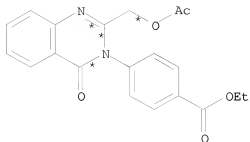


● Ag(I)

Q

2
STEPS
→

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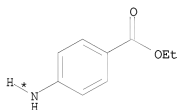


R
YIELD 82%

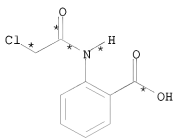
RX(1) RCT A 94-09-7, B 14422-49-2
RGT D 7719-12-2 PC13
PRO C 76535-04-1

RX(8) RCT Q 563-63-3, C 76535-04-1
PRO R 153705-99-8

RX(17) OF 17 COMPOSED OF RX(1), RX(9)
RX(17) A + B + S ==> T



A



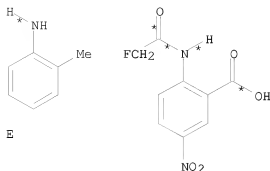
B



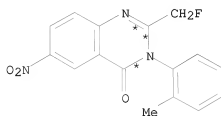
● Ag(I)

S

2
STEPS
=>



(2) →



YIELD 93%

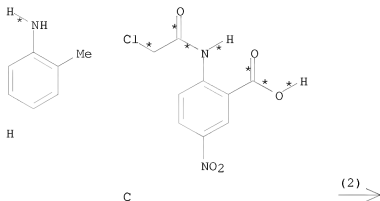
RX(2) RCT E 95-53-4, C 87266-10-2
 RGT G 7719-12-2 PC13
 PRO F 56287-73-1
 SOL 75-09-2 CH2C12

L3 ANSWER 139 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 119:95552 CASREACT
 TITLE: Preparation of quinazolinone derivative as an
 intermediate for afloqualone
 INVENTOR(S): Kamifuji, Tamiro; Matsui, Kozo; Okatake, Mitsuru
 PATENT ASSIGNEE(S): Sumika Fuain Kemu Kk, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05078333	A	19930330	JP 1991-86166	19910325
JP 2761677	B2	19980604		
PRIORITY APPLN. INFO.:			JP 1991-86166	19910325

AB 2-Fluoromethyl-3-(2-methylphenyl)-6-nitro-4(3H)-quinazolinone (I), useful as an intermediate for minor tranquilizing and muscle relaxing afloqualone, is prepared by treatment of 2-fluoroacetamido-5-nitrobenzoic acid (II) with o-toluidine. Treatment of 5-nitroanthranilic acid with AcNH₂, Me₃SiCl, and Et₃N in CH₂Cl₂ at .apprx.42° for 1 h, then with monofluoroacetyl chloride at .apprx.42° for 3 h gave 98.2% II, which was treated with o-toluidine and PCl₃ in CH₂Cl₂ at .apprx.40° for 9 h to afford 93.8% I.

RX(2) OF 3 ...H + C ==> I



I
YIELD 93%

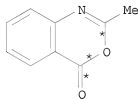
RX(2) RCT H 95-53-4, C 135590-27-1
RGT J 7719-12-2 PCl₃
PRO I 56287-73-1
SOL 75-09-2 CH₂Cl₂

AUTHOR(S): Abbady, M. S.
 CORPORATE SOURCE: Fac. Sci., Assiut Univ., Assiut, Egypt
 SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1992), 68(1-4), 69-76
 CODEN: PSSLEC; ISSN: 1042-6507
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

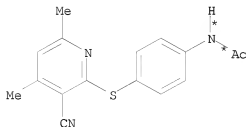
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Aminophenylthiopyridine I (R = NH₂) (II) was prepared by reaction of 2-chloro-3-cyano-4,6-dimethylpyridine and 4-bromonitrobenzene in aqueous sodium sulfide solution. Condensation of II with aromatic aldehydes, 2-methylbenzoxazin-4-one, azalactone and succinic anhydride afforded the expected products I (R = N:CHC₆H₄R₁, Q, Q1, Q2; R₁ = H, 4-NO₂, 4-NMe₂, 2-OH). Coupling of I (R = N:NC1) with active methylene compds. gave the corresponding hydrazones I (R = NHN:CR₂CO₂Et, R₂ = Ac, cyano). Cyclization of I (R = NHN:CacCO₂Et) with AlCl₃ gave the cinnoline derivative III which condensed with phenylhydrazine to give the pyrazolocinnoline derivative IV. Oxidation of some of the prepared sulfides with H₂O₂ in AcOH afforded the corresponding sulfones.

RX(9) OF 58 ...R + F ==> S...



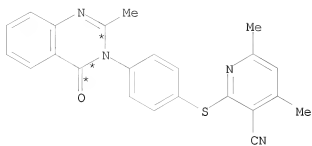
R



F

(9) →

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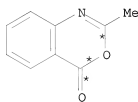


S
YIELD 58%

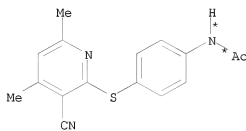
RX(9) RCT R 525-76-8, F 142531-61-1
PRO S 142531-65-5

RX(36) OF 58 COMPOSED OF RX(9), RX(10)

RX(36) R + F ==> T

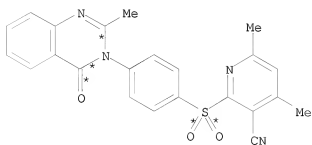


R



F

2
STEPS
→



T
YIELD 42%

RX(9) RCT R 525-76-8, F 142531-61-1
PRO S 142531-65-5

RX(10) RCT S 142531-65-5

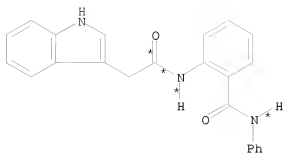
RGT H 7722-84-1 H2O2
PRO T 142531-66-6

L3 ANSWER 141 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 117:69809 CASREACT
TITLE: Synthesis and x-ray crystallographic analysis of
quinazolinone cholecystokinin/gastrin receptor ligands
AUTHOR(S): Yu, Melvin J.; McCowan, Jefferson R.; Mason, Norman
R.; Deeter, Jack B.; Mendelsohn, Laurane G.
CORPORATE SOURCE: Lilly Res. Lab., Eli Lilly Co., Indianapolis, IN,
46285, USA
SOURCE: Journal of Medicinal Chemistry (1992), 35(14), 2534-42
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

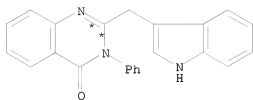
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. exemplified by 4(3H)-quinazolinone I (X = OCHMe₂, Y = Br, n = 2) (II) (IC₅₀ = 0.0093 μM using mouse brain membranes) represent a structurally novel series of non-peptide cholecystokinin B receptor ligands. Since asperlicin, a selective CCK-A receptor antagonist, may be regarded as a conformationally constrained 2-substituted-3-phenyl-4(3H)-quinazolinone, the progenitor of compound II, compound I (X = Y = H, n = 2), might therefore represent a conformationally flexible pharmacophore of the natural product. Quinazolinone derivs., e.g. I (X = Y = H; n = 1, 2, 3), III and IV (R = H, Me), were prepared in order to probe possible conformational preferences for this class of receptor ligands, in particular the spatial relationship between the indole and quinazolinone rings. Thus, anilide V was treated with 1,3-dioxane-4,6-dione VI in the presence of pyridium tosylate in pyridine to give IV (R = H). The x-ray crystal structure conformation for IV (R = H) (IC₅₀ = 0.026 μM) is extended with the two heteroarom. rings adopting an antiperiplanar arrangement around the central σ bond of the ethane linker, whereas the solid-state conformation for a less active analog III (IC₅₀ = 9.1 μM) is folded with the two heteroarom. systems adopting a synclinal orientation. However, MM2 force field calcns. (MacroModel, v 3.0) suggest that the energy difference between the folded and extended conformation is small and that other factors such as unfavorable steric interactions may account for the difference in receptor affinity. For derivs. with one or to three methylene units separating the indole and quinazolinone rings, maximal receptor binding activity was found when the distance separating the two heteroarom. systems is defined by an Et group. Introducing unsatn. into the ethylene bridge of II limited the conformational flexibility of the mol. and decreased its receptor affinity greater than 2 orders of magnitude.

RX(2) OF 17 ...F ==> G



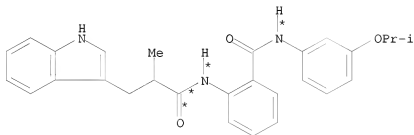
F

(2) \longrightarrow 

G

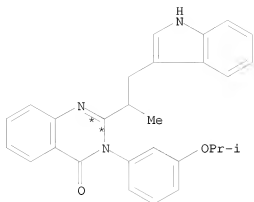
RX(2) RCT F 142005-24-1
 RGT H 104-15-4 TsOH
 PRO G 139571-49-6
 SOL 108-88-3 PhMe
 NIE Key step

RX(4) OF 17 ...L ==> O



L

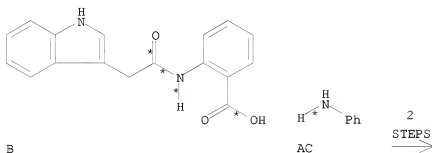
(4) \longrightarrow



O

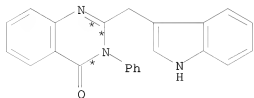
RX(4) RCT L 142005-17-2
 RGT P 24057-28-1 Pyridinium tosylate
 PRO O 142005-18-3
 SOL 110-86-1 Pyridine
 NTE Key step

RX(14) OF 17 COMPOSED OF RX(9), RX(2)
 RX(14) B + AC ==> G



B

AC



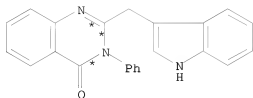
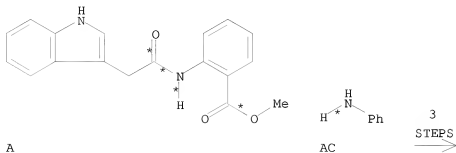
G

RX(9) RCT B 57932-49-7, AC 62-53-3
 RGT M 530-62-1 Diimidazolyl ketone, P 24057-28-1 Pyridinium tosylate
 PRO F 142005-24-1
 SOL 109-99-9 THF

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RX(2) RCT F 142005-24-1
RGT H 104-15-4 TsOH
PRO G 139571-49-6
SOL 108-88-3 PhMe
NTE Key step

RX(15) OF 17 COMPOSED OF RX(1), RX(9), RX(2)
RX(15) A + AC ==> G



RX(1) RCT A 139543-68-3
RGT C 1310-73-2 NaOH
PRO B 57932-49-7
SOL 7732-18-5 Water, 67-56-1 MeOH

RX(9) RCT B 57932-49-7, AC 62-53-3
RGT M 530-62-1 Diimidazolyl ketone, P 24057-28-1 Pyridinium tosylate
PRO F 142005-24-1
SOL 109-99-9 THF

RX(2) RCT F 142005-24-1
RGT H 104-15-4 TsOH
PRO G 139571-49-6
SOL 108-88-3 PhMe
NTE Key step

TITLE: The synthesis of some 3-amino-2-(halomethyl)-, 2-(halomethyl)-3-(substituted amino)- and 2-(halomethyl)-3-hetarylquinazolin-4(3H)-ones as potential plant protecting agents

AUTHOR(S): Fetter, Jozsef; Czuppon, Tibor; Hornyak, Gyula; Feller, Antal

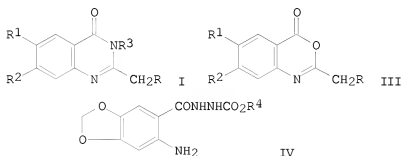
CORPORATE SOURCE: Dep. Org. Chem., Tech. Univ. Budapest, Budapest, H-1521, Hung.

SOURCE: Tetrahedron (1991), 47(45), 9393-410
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

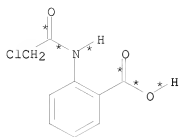
GI



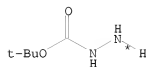
AB A series of quinazolinyl carbazates I [R = F, Cl, Br; R¹ = H, NO₂; R² = H or R¹R² = OCH₂O; R³ = NHCO₂Et, NHCO₂CMe₃ (II)] and hetaryl derivs. I (R¹ = 3,5-dimethyl-4-oxazolyl, 3,5-dimethyl-4-pyrazolyl) were obtained by reacting benzoxazinones III (R³ = NHCO₂CMe₃) with alkyl carbazates and hetaryl amines, resp. Some of the carbazates II were obtained alternatively by treatment of carbazate IV (R⁴ = Et, CMe₃) with haloacetyl halides. The tert-Bu carbazates I (R³ = NHCO₂CMe₃) were converted into amino quinazolinones I (R³ = NH₂), some of which were further converted into dimethylpyrrolyl derivs. I (R³ = 2,5-dimethyl-1-pyrrolyl). I (R³ = NH₂; R² = R¹ = H; R = Br) was obtained by brominating its 2-Me analog with cyanogen bromide. Biol. screening showed that some of the prepared quinazolines, namely I (R³ = NH₂; R¹ = R² = H; R = Cl) had a significant antifungal activity, while I (R³ = 3,5-dimethyl-4-pyrazolyl; R¹ = R² = H; R = F) had an effect on various functions of the CNS.

RX(53) OF 131 COMPOSED OF RX(7), RX(18)
RX(53) C + T ==> AC

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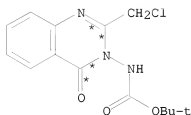


C



T

2
STEPS
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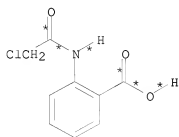
AC

YIELD 80%

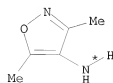
RX(7) RCT C 14422-49-2
RGT M 108-24-7 Ac2O
PRO L 98592-35-9

RX(18) RCT T 870-46-2, L 98592-35-9
PRO AC 138639-39-1

RX(54) OF 131 COMPOSED OF RX(7), RX(36)
RX(54) C + AT ==> AU



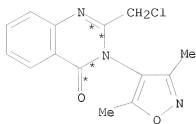
C



AT

2
STEPS
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10/ 562,112

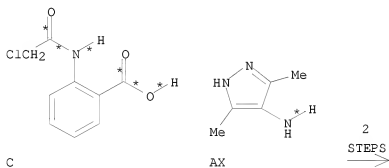


AU
YIELD 67%

RX(7) RCT C 14422-49-2
RGT M 108-24-7 Ac2O
PRO L 98592-35-9

RX(36) RCT AT 31329-64-3, L 98592-35-9
PRO AU 138639-52-8

RX(55) OF 131 COMPOSED OF RX(7), RX(39)
RX(55) C + AX ==> AY



AY
YIELD 67%

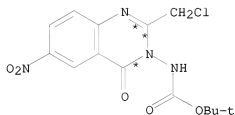
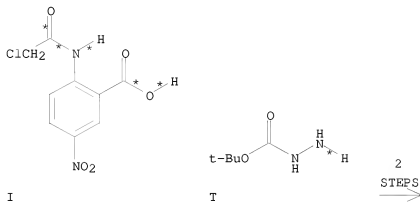
RX(7) RCT C 14422-49-2
RGT M 108-24-7 Ac2O

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PRO L 98592-35-9

RX(39) RCT AX 5272-86-6, L 98592-35-9
PRO AY 138639-56-2

RX(56) OF 131 COMPOSED OF RX(8), RX(19)
RX(56) I + T ==> AD

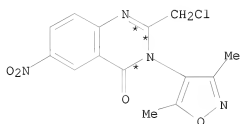
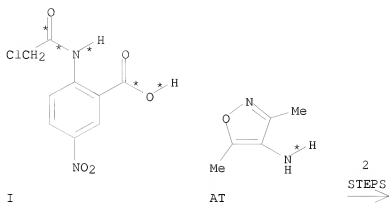


AD

RX(8) RCT I 135590-27-1
RGT M 108-24-7 Ac2O
PRO N 138639-61-9

RX(19) RCT T 870-46-2, N 138639-61-9
PRO AD 138639-41-5

RX(57) OF 131 COMPOSED OF RX(8), RX(37)
RX(57) I + AT ==> AV

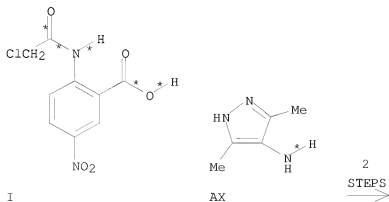


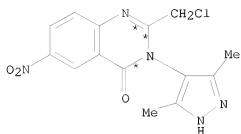
AV
YIELD 72%

RX(8) RCT I 135590-27-1
RGT M 108-24-7 Ac2O
PRO N 138639-61-9

RX(37) RCT AT 31329-64-3, N 138639-61-9
PRO AV 138639-53-9

RX(58) OF 131 COMPOSED OF RX(8), RX(40)
RX(58) I + AX ==> AZ



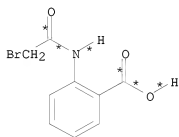


AZ
YIELD 81%

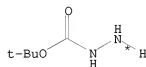
RX(8) RCT I 135590-27-1
RGT M 108-24-7 Ac2O
PRO N 138639-61-9

RX(40) RCT AX 5272-86-6, N 138639-61-9
PRO AZ 138639-58-4

RX(62) OF 131 COMPOSED OF RX(10), RX(22)
RX(62) E + T ==> AF

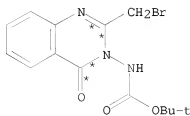


E



T

2
STEPS
=>



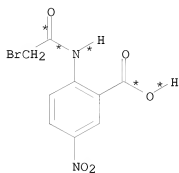
AF
YIELD 51%

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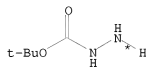
RX(10) RCT E 5979-85-1
 RGT M 108-24-7 Ac2O
 PRO P 43160-23-2

RX(22) RCT T 870-46-2, P 43160-23-2
 PRO AF 138639-40-4

RX(63) OF 131 COMPOSED OF RX(11), RX(25)
 RX(63) K + T ==> AH

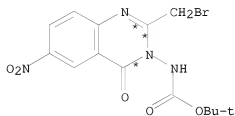


K



T

2
 STEPS
 >



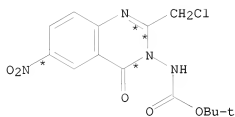
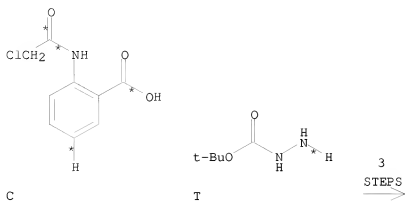
AH
 YIELD 55%

RX(11) RCT K 138639-68-6
 RGT M 108-24-7 Ac2O
 PRO Q 138639-62-0

RX(25) RCT T 870-46-2, Q 138639-62-0
 PRO AH 138639-42-6

RX(92) OF 131 COMPOSED OF RX(5), RX(8), RX(19)
 RX(92) C + T ==> AD

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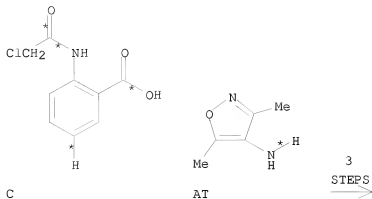
RX(5) RCT C 14422-49-2
RGT J 7697-37-2 HNO3
PRO I 135590-27-1

RX(8) RCT I 135590-27-1
RGT M 108-24-7 Ac2O
PRO N 138639-61-9

RX(19) RCT T 870-46-2, N 138639-61-9
PRO AD 138639-41-5

RX(93) OF 131 COMPOSED OF RX(5), RX(8), RX(37)

RX(93) C + AT ==> AV



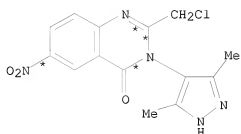
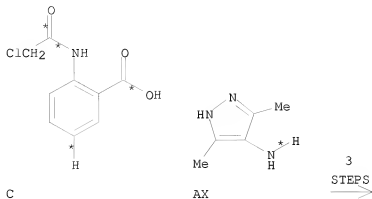
AV
YIELD 72%

RX(5) RCT C 14422-49-2
RGT J 7697-37-2 HNO3
PRO I 135590-27-1

RX(8) RCT I 135590-27-1
RGT M 108-24-7 Ac2O
PRO N 138639-61-9

RX(37) RCT AT 31329-64-3, N 138639-61-9
PRO AV 138639-53-9

RX(94) OF 131 COMPOSED OF RX(5), RX(8), RX(40)
RX(94) C + AX ==> AZ



YIELD 81%

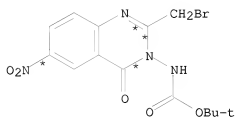
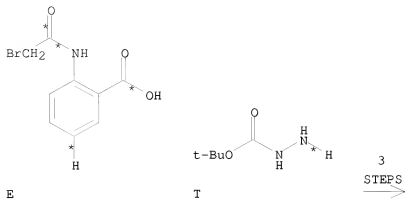
RX(5) RCT C 14422-49-2
RGT J 7697-37-2 HNO3
PRO I 135590-27-1

RX(8) RCT I 135590-27-1
RGT M 108-24-7 Ac2O
PRO N 138639-61-9

RX(40) RCT AX 5272-86-6, N 138639-61-9
PRO AZ 138639-58-4

RX(98) OF 131 COMPOSED OF RX(6), RX(11), RX(25)

RX(98) E + T ==> AH



AH
YIELD 55%

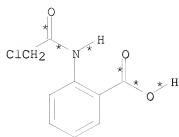
RX(6) RCT E 5979-85-1
RGT J 7697-37-2 HNO3
PRO K 138639-68-6

RX(11) RCT K 138639-68-6
RGT M 108-24-7 Ac2O
PRO Q 138639-62-0

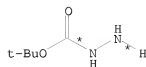
RX(25) RCT T 870-46-2, Q 138639-62-0
PRO AH 138639-42-6

RX(100) OF 131 COMPOSED OF RX(7), RX(18), RX(26)
RX(100) C + T ==> AI

10/ 562,112

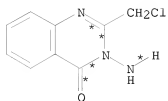


C



T

3
STEPS
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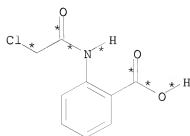
AI
YIELD 70%

RX(7) RCT C 14422-49-2
RGT M 108-24-7 Ac2O
PRO L 98592-35-9

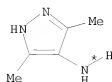
RX(18) RCT T 870-46-2, L 98592-35-9
PRO AC 138639-39-1

RX(26) RCT AC 138639-39-1
RGT AJ 64-19-7 AcOH
PRO AI 138639-45-9

RX(101) OF 131 COMPOSED OF RX(7), RX(39), RX(44)
RX(101) C + AX ==> BE

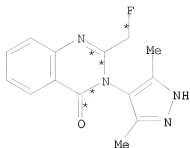


C



AX

3
STEPS
➞



BE

YIELD 31%

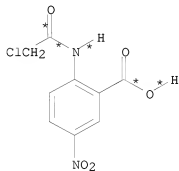
RX(7) RCT C 14422-49-2
 RGT M 108-24-7 Ac2O
 PRO L 98592-35-9

RX(39) RCT AX 5272-86-6, L 98592-35-9
 PRO AY 138639-56-2

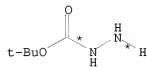
RX(44) RCT AY 138639-56-2
 RGT BC 7789-23-3 KF
 PRO BE 138639-57-3

RX(104) OF 131 COMPOSED OF RX(8), RX(19), RX(29)

RX(104) I + T ==> AN



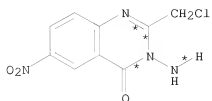
I



T

3
 STEPS
 →

10/ 562,112



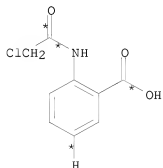
AN
YIELD 57%

RX(8) RCT I 135590-27-1
RGT M 108-24-7 Ac2O
PRO N 138639-61-9

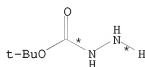
RX(19) RCT T 870-46-2, N 138639-61-9
PRO AD 138639-41-5

RX(29) RCT AD 138639-41-5
PRO AN 138639-46-0

RX(105) OF 131 COMPOSED OF RX(5), RX(8), RX(19), RX(29)
RX(105) C + T ==> AN

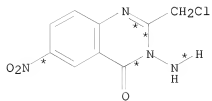


C



T

4
STEPS
→



AN
YIELD 57%

10/ 562,112

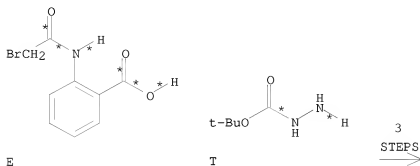
RX(5) RCT C 14422-49-2
RGT J 7697-37-2 HNO3
PRO I 135590-27-1

RX(8) RCT I 135590-27-1
RGT M 108-24-7 Ac2O
PRO N 138639-61-9

RX(19) RCT T 870-46-2, N 138639-61-9
PRO AD 138639-41-5

RX(29) RCT AD 138639-41-5
PRO AN 138639-46-0

RX(110) OF 131 COMPOSED OF RX(10), RX(22), RX(28)
RX(110) E + T ==> AL



AL
YIELD 56%

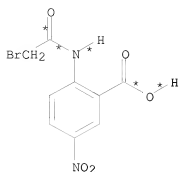
RX(10) RCT E 5979-85-1
RGT M 108-24-7 Ac2O
PRO P 43160-23-2

RX(22) RCT T 870-46-2, P 43160-23-2
PRO AF 138639-40-4

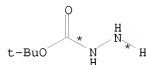
RX(28) RCT AF 138639-40-4
RGT AJ 64-19-7 AcOH
PRO AL 138639-34-6

RX(112) OF 131 COMPOSED OF RX(11), RX(25), RX(31)
RX(112) K + T ==> AO

10/ 562,112

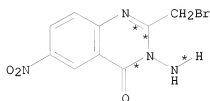


K



T

3
STEPS
→



AO

YIELD 76%

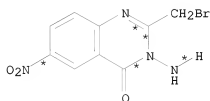
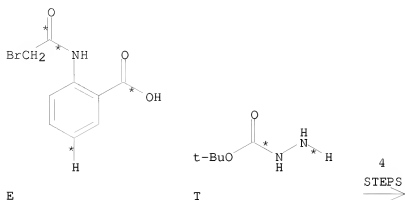
RX(11) RCT K 138639-68-6
RGT M 108-24-7 Ac₂O
PRO Q 138639-62-0

RX(25) RCT T 870-46-2, Q 138639-62-0
PRO AH 138639-42-6

RX(31) RCT AH 138639-42-6
RGT AJ 64-19-7 AcOH
PRO AO 138639-47-1

RX(113) OF 131 COMPOSED OF RX(6), RX(11), RX(25), RX(31)

RX(113) E + T ==> AO



AO
YIELD 76%

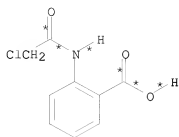
RX(6) RCT E 5979-85-1
 RGT J 7697-37-2 HNO3
 PRO K 138639-68-6

RX(11) RCT K 138639-68-6
 RGT M 108-24-7 Ac2O
 PRO Q 138639-62-0

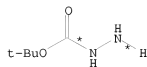
RX(25) RCT T 870-46-2, Q 138639-62-0
 PRO AH 138639-42-6

RX(31) RCT AH 138639-42-6
 RGT AJ 64-19-7 AcOH
 PRO AO 138639-47-1

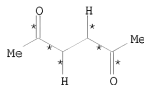
RX(124) OF 131 COMPOSED OF RX(7), RX(18), RX(26), RX(35)
RX(124) C + T + AR ==> AS



C

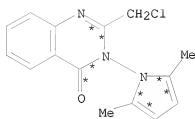


T



AR

4
STEPS
→



AS

YIELD 67%

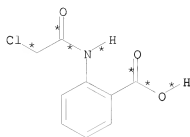
RX(7) RCT C 14422-49-2
RGT M 108-24-7 Ac2O
PRO L 98592-35-9

RX(18) RCT T 870-46-2, L 98592-35-9
PRO AC 138639-39-1

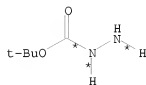
RX(26) RCT AC 138639-39-1
RGT AJ 64-19-7 AcOH
PRO AI 138639-45-9

RX(35) RCT AR 110-13-4, AI 138639-45-9
PRO AS 138639-50-6

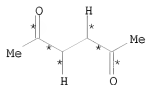
RX(130) OF 131 COMPOSED OF RX(7), RX(18), RX(26), RX(35), RX(42)
RX(130) C + T + AR ==> BB



C

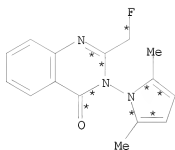


T



AR

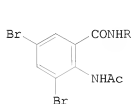
5
STEPS
→



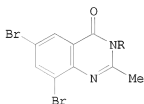
BB
YIELD 27%

RX(7)	RCT	C 14422-49-2
	RGT	M 108-24-7 Ac2O
	PRO	L 98592-35-9
RX(18)	RCT	T 870-46-2, L 98592-35-9
	PRO	AC 138639-39-1
RX(26)	RCT	AC 138639-39-1
	RGT	AJ 64-19-7 AcOH
	PRO	AI 138639-45-9
RX(35)	RCT	AR 110-13-4, AI 138639-45-9
	PRO	AS 138639-50-6
RX(42)	RCT	AS 138639-50-6
	RGT	BC 7789-23-3 KF
	PRO	BB 138639-51-7

L3 ANSWER 143 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 116:151715 CASREACT
 TITLE: Factors affecting cyclization of N-substituted
 2-acylamino-3,5-dibromobenzamides to 2,3-disubstituted
 6,8-dibromoquinazolin-4-ones
 AUTHOR(S): Ismail, M. Fekry; Emara, Samir A.; Enayat, E. I.;
 Mustafa, Omina E. A.
 CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
 SOURCE: Polish Journal of Chemistry (1991), 65(7-8), 1259-63
 CODEN: PJCHDQ; ISSN: 0137-5083
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



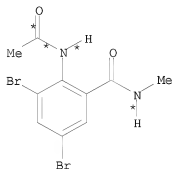
I



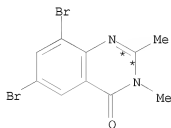
II

AB Cyclization of (acetyl amino)dibromobenzamides I (R = Me, CH₂Ph, Ph) in the presence of an amine base gave quinazolinones II. The cyclization process was dependent on basicity of the base, polarity of the medium, reaction time, and the nature of the N-substituent.

RX(3) OF 7 ...C ==> F



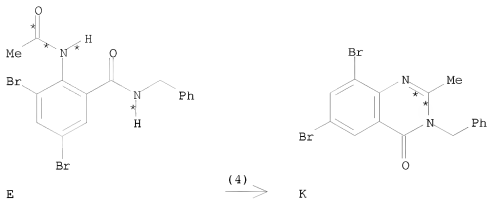
C



F

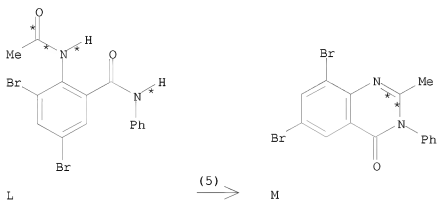
RX(3) RCT C 86993-54-6
 RGT G 75-04-7 EtNH₂, H 109-89-7 Et₂NH, I 121-44-8 Et₃N, J 1310-73-2
 NaOH
 PRO F 86993-61-5
 NTE DITRI

RX(4) OF 7 ...E ==> K



RX(4) RCT E 86993-56-8
 RGT G 75-04-7 EtNH₂, H 109-89-7 Et₂NH, I 121-44-8 Et₃N, J 1310-73-2 NaOH
 PRO K 86993-63-7
 NTE DITRI

RX(5) OF 7 L ==> M



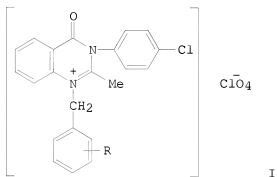
RX(5) RCT L 78993-24-5
 RGT G 75-04-7 EtNH₂, H 109-89-7 Et₂NH, I 121-44-8 Et₃N, J 1310-73-2 NaOH
 PRO M 4145-21-5
 NTE DITRI

L3 ANSWER 144 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 116:143879 CASREACT
 TITLE: Benzyl phenyl quiazolinone perchlorates displaying
 analgesic, anticonvulsive, and antimicrobial activity
 Chernobrovin, N. I.; Kozhevnikov, Yu. V.; Morozova, G.
 E.; Zalesov, V. S.; Plaksina, A. N.

PATENT ASSIGNEE(S): Perm Pharmaceutical Institute, USSR
 SOURCE: U.S.S.R. From: Otkrytiya, Izobret. 1991, (28), 258.
 CODEN: URXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Russian
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

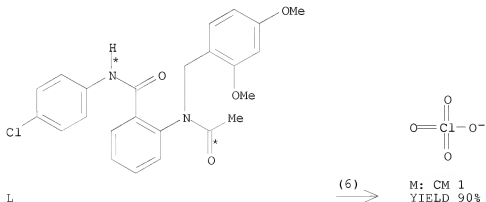
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 1110140	A1	19910730	SU 1983-3554870	19830217

PRIORITY APPLN. INFO.:
 GI

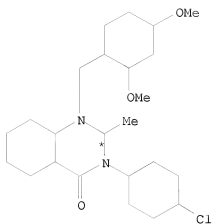


AB The title compds. [I: R = (OCH3)2] display analgesic, anticonvulsive, and antimicrobial activity.

RX(6) OF 14 L ==> M



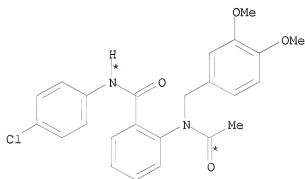
10/ 562,112



M: CM 2
YIELD 90%

RX(6) RCT L 143424-27-5
 RGT N 7601-90-3 HClO4
 PRO M 139755-24-1

RX(7) OF 14 ...K ==> O

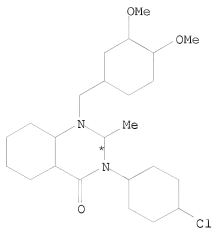


K

(7) ➔



O: CM 1
YIELD 84%



O: CM 2
YIELD 84%

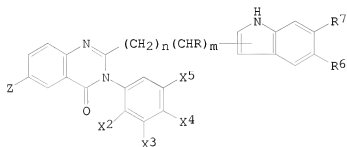
RX(7) RCT K 143424-31-1
RGT N 7601-90-3 HC104
PRO O 143579-10-6

L3 ANSWER 145 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 116:128964 CASREACT
TITLE: Preparation of 2-indolyl-3-phenyl-4-quinazolinones as
cholecystokinin antagonists
INVENTOR(S): Yu, Melvin J.; Mccowan, Jefferson R.; Thrasher, K.
Jeff
PATENT ASSIGNEE(S): Eli Lilly and Co., USA
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

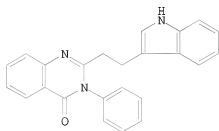
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
US 5075313	A	19911224	US 1990-581943	19900913
CA 2050994	A1	19920314	CA 1991-2050994	19910909
ZA 9107149	A	19920527	ZA 1991-7149	19910909
JP 04247080	A	19920903	JP 1991-227902	19910909
FI 9104262	A	19920314	FI 1991-4262	19910910
HU 59128	A2	19920428	HU 1991-2921	19910910
NO 9103579	A	19920316	NO 1991-3579	19910911
AU 9183829	A	19920319	AU 1991-83829	19910911
AU 641043	B2	19930909		
CZ 279774	B6	19950614	CZ 1991-2799	19910911
EP 475755	A1	19920318	EP 1991-308324	19910912
EP 475755	B1	19950927		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE

CN 1059722	A	19920325	CN 1991-108887	19910912
ES 2078455	T3	19951216	ES 1991-308324	19910912
US 5196427	A	19930323	US 1991-763104	19910920
PRIORITY APPLN. INFO.:			US 1990-581943	19900913
OTHER SOURCE(S):	MARPAT 116:128964			
GI				



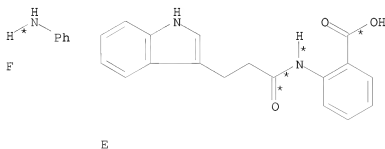
I



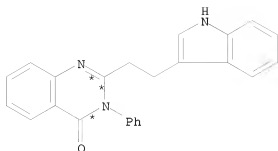
II

AB Title compds. (I; $n = 1, 2$; $m = 0, 1$; $R = H$, alkyl, $PhCH_2$, Ph ; $Z = H$, halo; $X_2-X_5 = H$, halo, CF_3 , alkoxy, alkyl, alkylthio, amino; $R_6, R_7 = H$, alkyl, alkoxy, halo, CF_3), were prepared. Thus, 3-(3-indolyl)propionic acid and Me anthranilate in THF were refluxed with carbonyldiimidazole and pyridinium p-toluenesulfonate to give 70% 3-(3-indolyl)-N-(2-methoxycarbonylphenyl)propionamide. This was saponified with $NaOH/MeOH$ followed by treatment with aniline, carbonyldiimidazole, and pyridinium p-toluenesulfonate in refluxing THF to give title compound II. I bound to CCK receptors in mouse brain membrane preps. with IC_{50} 's of 0.019-1.2 μM . I are useful in treating gastrointestinal, CNS, and appetite disorders.

RX(3) OF 6 ...F + E ==> G



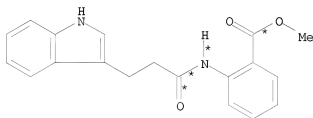
(3) →



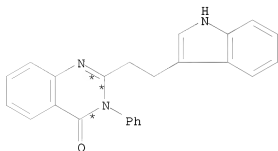
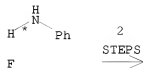
G

RX(3) RCT F 62-53-3, E 139543-67-2
 PRO G 133040-57-0
 CAT 530-62-1 Diimidazolyl ketone

RX(5) OF 6 COMPOSED OF RX(2), RX(3)
 RX(5) C + F ==> G



C



G

RX(2) RCT C 139543-66-1
 PRO E 139543-67-2
 RX(3) RCT F 62-53-3, E 139543-67-2

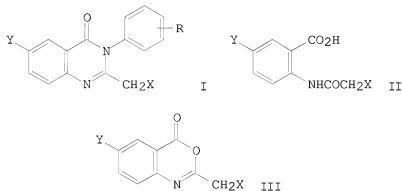
PRO G 133040-57-0
 CAT 530-62-1 Diimidazolyl ketone

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 146 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 115:114535 CASREACT
 TITLE: Preparation of quinazolinone derivatives as intermediates for minor tranquilizers and neuroleptics
 INVENTOR(S): Myashita, Masahiko
 PATENT ASSIGNEE(S): Nippon Synthetic Chemical Industry Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03058977	A	19910314	JP 1989-196366	19890727

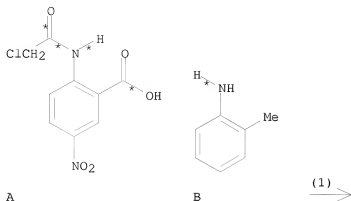
PRIORITY APPLN. INFO.: JP 1989-196366 19890727
 OTHER SOURCE(S): MARPAT 115:114535
 GI



AB The title derivs. I (R = alkyl; X = halo; Y = alkyl, halo, alkylamino, NO₂), useful as intermediates for I (X = F; Y = NH₂) which are minor tranquilizers and neuroleptics, are prepared by cyclization of N-acylanthranilic acids II (X, Y = same as I) with Ac₂O at a mol ratio of 1:(0.9-1.2) and treatment of the resulting benzoxazinones III (X, Y = same as I) with RC₆H₄NH₂ without further purification. Thus, a solution of 0.023 mol II (X = Cl, Y = NO₂) in toluene was refluxed with 0.025 mol Ac₂O for 6 h and further refluxed with o-MeC₆H₄NH₂ for 3 h to give 87% I (R = 2-Me, X = Cl, Y = NO₂).

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RX(1) OF 1 A + B ==> C



C
YIELD 87%

RX(1) RCT A 135590-27-1

STAGE(1)

RGT D 108-24-7 Ac2O

SOL 108-88-3 PhMe

STAGE(2)

RCT B 95-53-4

PRO C 61899-76-1

L3 ANSWER 147 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:

115:29242 CASREACT

TITLE:

A new synthesis of
2-aryl-2H-pyrazino[2,1-b]quinazoline-3,6(1H,4H)-diones
Reddy, P. S. N.; Nagaraju, C.

AUTHOR(S):

CORPORATE SOURCE:

Dep. Chem., Osmania Univ., Hyderabad, 500 007, India

SOURCE:

Synthetic Communications (1991), 21(2), 173-81

CODEN: SYNCAV; ISSN: 0039-7911

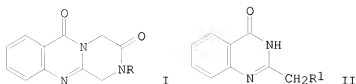
DOCUMENT TYPE:

Journal

LANGUAGE:

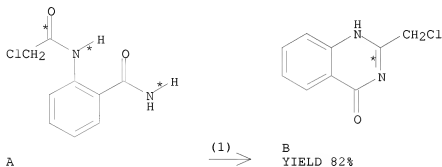
English

GI



AB Six title compds. I (R = Ph, substituted Ph) were prepared starting from (2-chloromethyl)quinazolinone II (R1 = Cl) in 3 steps involving condensation with RNH2 to give II (R1 = NHR), condensation with chloroacetic anhydride or ClCH2COCl to give II (R1 = NRCOCH2Cl) and dehydrochlorination-cyclization with Et3N in dioxane at room temperature

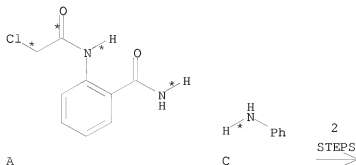
RX(1) OF 19 A ==> B...



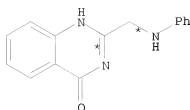
RX(1) RCT A 21721-78-8
 PRO B 3817-05-8
 NTE Polyphosphate Et ester solvent

RX(8) OF 19 COMPOSED OF RX(1), RX(2)

RX(8) A + C ==> D



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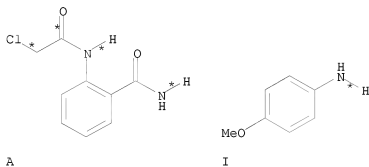


D
YIELD 52%

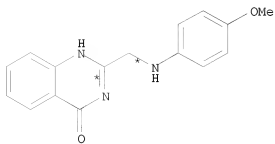
RX(1) RCT A 21721-78-8
PRO B 3817-05-8
NTE Polyphosphate Et ester solvent

RX(2) RCT B 3817-05-8, C 62-53-3
PRO D 3817-06-9
SOL 64-17-5 EtOH

RX(9) OF 19 COMPOSED OF RX(1), RX(4)
RX(9) A + I ==> J



2
STEPS
→



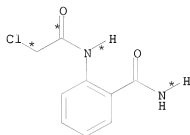
J
YIELD 42%

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RX(1) RCT A 21721-78-8
 PRO B 3817-05-8
 NTE Polyphosphate Et ester solvent

RX(4) RCT B 3817-05-8, I 104-94-9
 PRO J 134577-52-9
 SOL 64-17-5 EtOH

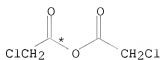
RX(14) OF 19 COMPOSED OF RX(1), RX(2), RX(3)
 RX(14) A + C + F ==> G



A

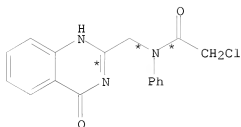


C



F

3
 STEPS
 →



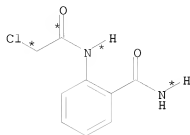
G
 YIELD 72%

RX(1) RCT A 21721-78-8
 PRO B 3817-05-8
 NTE Polyphosphate Et ester solvent

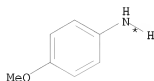
RX(2) RCT B 3817-05-8, C 62-53-3
 PRO D 3817-06-9
 SOL 64-17-5 EtOH

RX(3) RCT D 3817-06-9, F 541-88-8
 PRO G 134577-55-2
 SOL 75-09-2 CH2Cl2

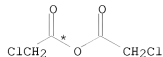
RX(15) OF 19 COMPOSED OF RX(1), RX(4), RX(6)
 RX(15) A + I + F ==> N



A

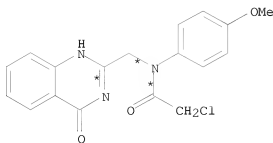


I



F

3
 STEPS
 →



N
 YIELD 84%

RX(1)	RCT	A 21721-78-8
	PRO	B 3817-05-8
	NTE	Polyphosphate Et ester solvent
RX(4)	RCT	B 3817-05-8, I 104-94-9
	PRO	J 134577-52-9
	SOL	64-17-5 EtOH
RX(6)	RCT	J 134577-52-9, F 541-88-8
	PRO	N 134577-58-5
	SOL	75-09-2 CH2Cl2

TITLE: Synthesis and reactions of
2-(α -benzoylamino-p-chlorostyryl)-3,1(4H)-
benzoxazin-4-one with some nucleophilic reagents:
synthesis of quinazolinone, tetrazole and
benzimidazole derivatives

AUTHOR(S): El-Khamry, Abdel Momen A.; El-Nagdy, S.; Shaban, M. E.

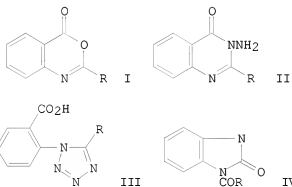
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt

SOURCE: Egyptian Journal of Chemistry (1990), Volume Date
1988, 31(2), 261-9
CODEN: EGJCA3; ISSN: 0367-0422

DOCUMENT TYPE: Journal

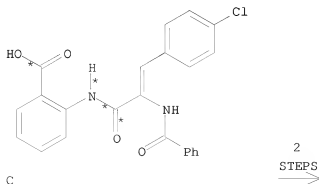
LANGUAGE: English

GI

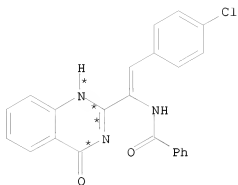


AB Treating benzoxazinone I (R = p-ClC₆H₄CH:CNHBz throughout) with R₁NH₂ (R₁ = Et, PhCH₂, 4-pyridyl, p-tolyl, p-MeOC₆H₄, NH₂, PhNH) gave 60-85% o-R₁NHCOC₆H₄NHCOR. Treating I with N₂H₄ in BuOH gave 65% quinazolinone II which condensed with R₂CHO (R₂ = p-ClC₆H₄, p-O₂NC₆H₄, p-Me₂NC₆H₄) gave 60-70% of the corresponding Schiff bases. Addnl. obtained was tetrazole III and benzimidazolone IV.

RX(34) OF 71 COMPOSED OF RX(3), RX(13)
RX(34) C ==> Y



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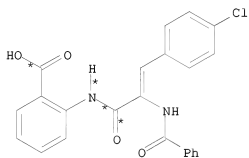


Y

RX(3) RCT C 132994-47-9
 PRO D 132994-48-0
 CAT 108-24-7 Ac2O

RX(13) RCT D 132994-48-0
 PRO Y 132994-58-2
 CAT 631-61-8 NH4OAc

RX(35) OF 71 COMPOSED OF RX(3), RX(14)
 RX(35) C + AA ==> Y

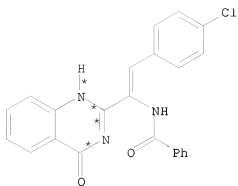


C



AA

2
 STEPS
 >

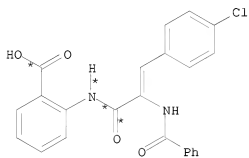


Y

RX(3) RCT C 132994-47-9
 PRO D 132994-48-0
 CAT 108-24-7 Ac2O

RX(14) RCT D 132994-48-0, AA 75-12-7
 PRO Y 132994-58-2

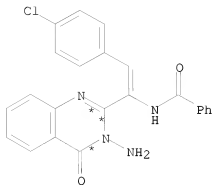
RX(36) OF 71 COMPOSED OF RX(3), RX(15)
 RX(36) C ==> AB



C

2
 STEPS
 →

10/ 562,112



AB

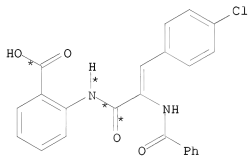
YIELD 65%

RX(3) RCT C 132994-47-9
 PRO D 132994-48-0
 CAT 108-24-7 Ac2O

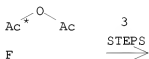
RX(15) RCT D 132994-48-0
 RGT R 302-01-2 N2H4
 PRO AB 132994-59-3

RX(59) OF 71 COMPOSED OF RX(3), RX(15), RX(16)

RX(59) C + F ==> AC

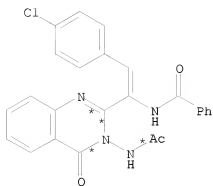


C



F

3
 STEPS
 →



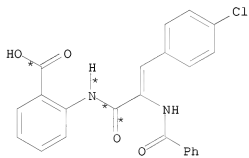
AC

RX(3) RCT C 132994-47-9
 PRO D 132994-48-0
 CAT 108-24-7 Ac2O

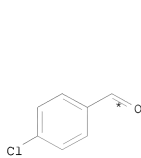
RX(15) RCT D 132994-48-0
 RGT R 302-01-2 N2H4
 PRO AB 132994-59-3

RX(16) RCT AB 132994-59-3, F 108-24-7
 PRO AC 132994-60-6

RX(60) OF 71 COMPOSED OF RX(3), RX(15), RX(17)
 RX(60) C + AD ==> AE

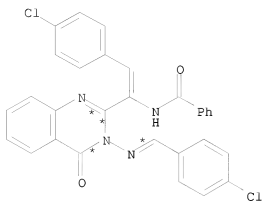


C



AD

3
 STEPS
 ➞



AE

YIELD 65%

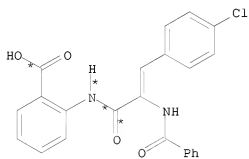
RX(3) RCT C 132994-47-9
 PRO D 132994-48-0
 CAT 108-24-7 Ac2O

RX(15) RCT D 132994-48-0
 RGT R 302-01-2 N2H4
 PRO AB 132994-59-3

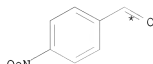
RX(17) RCT AB 132994-59-3, AD 104-88-1
 PRO AE 132994-61-7

RX(61) OF 71 COMPOSED OF RX(3), RX(15), RX(18)

RX(61) C + AF ==> AG

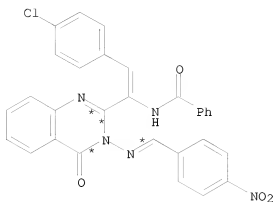


C



AF

3
 STEPS
 →



AG

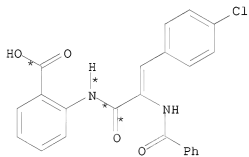
YIELD 60%

RX(3) RCT C 132994-47-9
PRO D 132994-48-0
CAT 108-24-7 Ac2O

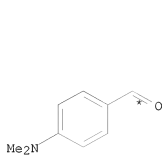
RX(15) RCT D 132994-48-0
RGT R 302-01-2 N2H4
PRO AB 132994-59-3

RX(18) RCT AB 132994-59-3, AF 555-16-8
PRO AG 132994-62-8

RX(62) OF 71 COMPOSED OF RX(3), RX(15), RX(19)
RX(62) C + AH ==> AI

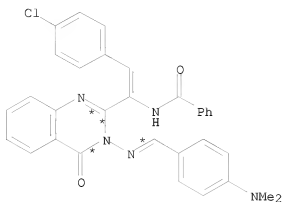


C



AH

3
STEPS
→



AI
YIELD 70%

RX(3) RCT C 132994-47-9
PRO D 132994-48-0
CAT 108-24-7 Ac2O

RX(15) RCT D 132994-48-0
RGT R 302-01-2 N2H4
PRO AB 132994-59-3

RX(19) RCT AB 132994-59-3, AH 100-10-7
PRO AI 133023-95-7

L3 ANSWER 149 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 114:163892 CASREACT

TITLE: Synthesis of 2-alkyl-3-aminoquinazolin-4(3H)-ones and their use for enantioselective aminoaziridinations using a chiral oxidant

AUTHOR(S): Zhalnina, G. V.; Kuznetsov, M. A.; Semenovskii, V. V.; Shustov, G. V.

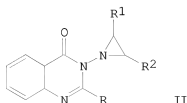
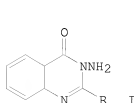
CORPORATE SOURCE: USSR

SOURCE: Vestnik Leningradskogo Universiteta, Seriya 4: Fizika, Khimiya (1990), (3), 72-6
CODEN: VLUFBI; ISSN: 0024-0826

DOCUMENT TYPE: Journal

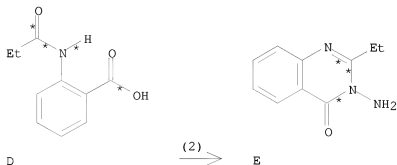
LANGUAGE: Russian

GI



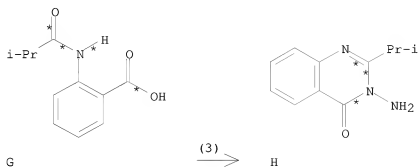
AB Aminoquinazolinone derivs. (I; R = Et, CHMe2, CMe3) were prepared from anthranilic acid Me ester. Oxidation of (I; R = Et, CHMe2) by Pb(OAc)₄ in the presence of excess styrene, trans-stilbene or dimethyl fumarate affords the corresponding racemic dihydroquinazolinylaziridines (II; R₁ = Ph, CO₂Me; R₂ = H, Ph, CO₂Me) in 50-70% yield. With optically active oxidant lead tetra-(S)-2-methylbutanoate, asym. induction is observed only for trans-stilbene.

RX(2) OF 11 ...D ==> E



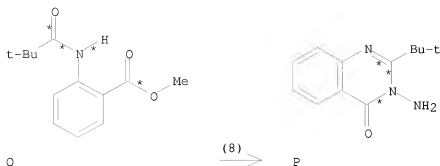
RX(2) RCT D 19165-26-5
RGT F 302-01-2 N2H4
PRO E 50547-51-8

RX(3) OF 11 ...G ==> H



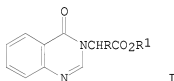
RX(3) RCT G 17840-96-9
RGT F 302-01-2 N2H4
PRO H 70589-51-4

RX(8) OF 11 ...O ==> P



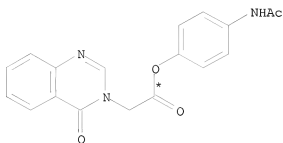
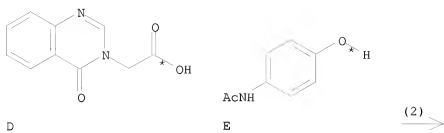
RX(8) RCT O 84540-62-5
 RGT F 302-01-2 N2H4
 PRO P 132871-77-3

L3 ANSWER 150 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 114:81745 CASREACT
 TITLE: Esters of quinazolin-4[3H]-on-3-ylacetic and
 2-(quinazolin-4[3H]-on-3-yl)propionic acids
 AUTHOR(S): Fisnerova, L.; Brunova, B.; Maturova, E.; Grimova, J.
 CORPORATE SOURCE: Vyzk. Ustav Farm. Biochem., Prague, Czech.
 SOURCE: Cesko-Slovenska Farmacie (1990), 39(6), 275-7
 CODEN: CKFRAY; ISSN: 0009-0530
 DOCUMENT TYPE: Journal
 LANGUAGE: Czech
 GI



AB Several new esters of quinazolinonylacetic I ($\text{R} = \text{H}$; $\text{R}^1 =$ 2-benzimidazolylhydroxymethyl, 4-AcNHC6H4, substituted biphenylol) and quinazolinonylpropionic I ($\text{R} = \text{Me}$, $\text{R}^1 =$ 2-benzimidazolylhydroxymethyl, 4-AcNHC6H4) acid were prepared. The analgetic efficacy of these compds. was comparable to that of aminophenazone, while their acute toxicity in mice was significantly lower.

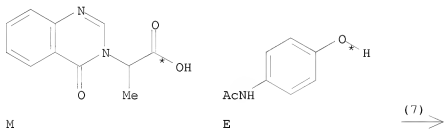
RX(2) OF 8 D + E ==> F

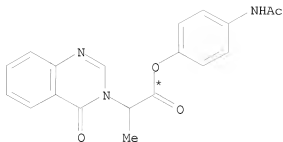


F
YIELD 60%

RX(2) RCT D 14663-53-7, E 103-90-2
 PRO F 131842-95-0

RX(7) OF 8 M + E \implies N

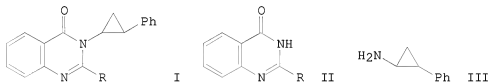




N
YIELD 48%

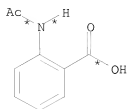
RX(7) RCT M 61381-36-0, E 103-90-2
PRO N 131843-00-0

L3 ANSWER 151 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 114:62036 CASREACT
TITLE: Some 4-(3H)-quinazolinones as anticonvulsants and
monoamine oxidase inhibitors
AUTHOR(S): Aboul-Enein, M. Nabil; Eid, A. I.; El-Azzouny, Aida A.
CORPORATE SOURCE: Lab. Pharm. Sci., Natl. Res. Cent., Cairo, Egypt
SOURCE: Egyptian Journal of Chemistry (1989), Volume Date
1987, 30(6), 515-16
CODEN: EGJCA3; ISSN: 0367-0422
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Phenylcyclopropylquinazolinones I (R = Me, Ph) were prepared by the reaction of quinazolinones II with phenylcyclopropylamine III. Various derivs., e.g., I (R = CH:CHR1 = Ph, substituted Ph) of I (R = Me) were prepared by condensation with aldehydes.

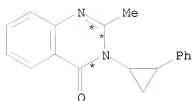
RX(1) OF 12 A + B ==> C...



A



B

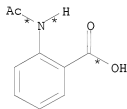
(1) \longrightarrow 

C

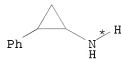
YIELD 50%

RX(1) RCT A 89-52-1, B 54-97-7
PRO C 131557-26-1

RX(8) OF 12 COMPOSED OF RX(1), RX(2)
RX(8) A + B + D \implies E



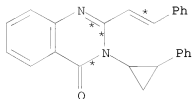
A



B



D

2
STEPS
 \longrightarrow 

E

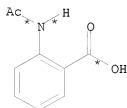
YIELD 82%

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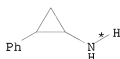
RX(1) RCT A 89-52-1, B 54-97-7
PRO C 131557-26-1

RX(2) RCT C 131557-26-1, D 100-52-7
PRO E 131557-28-3

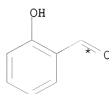
RX(9) OF 12 COMPOSED OF RX(1), RX(3)
RX(9) A + B + F ==> G



A

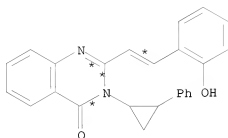


B



F

2
STEPS
→



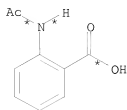
G

YIELD 75%

RX(1) RCT A 89-52-1, B 54-97-7
PRO C 131557-26-1

RX(3) RCT C 131557-26-1, F 90-02-8
PRO G 131557-29-4

RX(10) OF 12 COMPOSED OF RX(1), RX(4)
RX(10) A + B + H ==> I



A

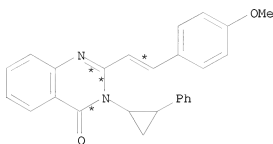


B



H

2
STEPS
→



I

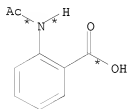
YIELD 78%

RX(1) RCT A 89-52-1, B 54-97-7
PRO C 131557-26-1

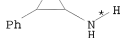
RX(4) RCT C 131557-26-1, H 123-11-5
PRO I 131557-30-7

RX(11) OF 12 COMPOSED OF RX(1), RX(5)

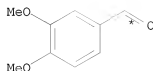
RX(11) A + B + J ==> K



A

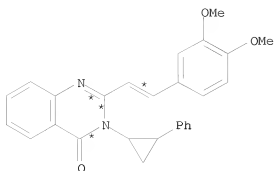


B



J

2
STEPS
→

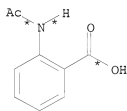


K

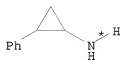
RX(1) RCT A 89-52-1, B 54-97-7
PRO C 131557-26-1

RX(5) RCT C 131557-26-1, J 120-14-9
PRO K 131557-31-8
CAT 110-86-1 Pyridine

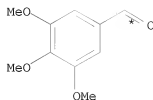
RX(12) OF 12 COMPOSED OF RX(1), RX(6)
RX(12) A + B + M ==> N



A

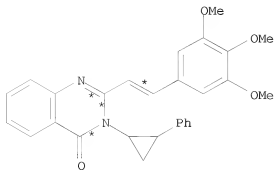


B



M

2
STEPS
→

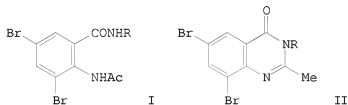


N

RX(1) RCT A 89-52-1, B 54-97-7
 PRO C 131557-26-1

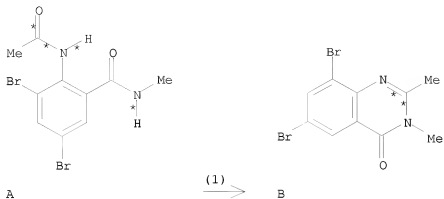
RX(6) RCT C 131557-26-1, M 86-81-7
 PRO N 131557-32-9
 CAT 110-86-1 Pyridine

L3 ANSWER 152 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 114:23917 CASREACT
 TITLE: Factors affecting cyclization of N-substituted
 2-(acetylamino)-3,5-dibromobenzamide to
 2,3-disubstituted 6,8-dibromoquinazolin-4-ones
 AUTHOR(S): Ismail, M. Fekry; Emara, Samir A.; Enayat, E. I.;
 Mustafa, Omnia E. A.
 CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
 SOURCE: Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (1990),
 29B(9), 811-13
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



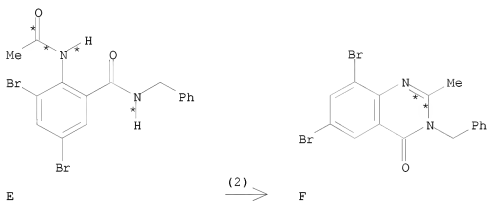
AB Factors affecting cyclization of (benzamide I (R = Me, Ph, PhCH₂) to the corresponding II were studied. The cyclization process depended on the basicity of the medium, time of reaction, polarity of solvent used as well as the nature of the substituents present.

RX(1) OF 3 A ==> B



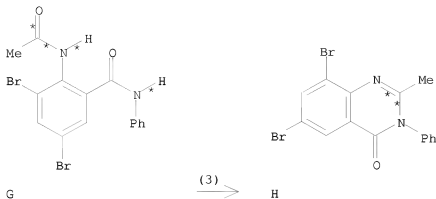
RX(1) RCT A 86993-54-6
 RGT C 75-04-7 EtNH₂
 PRO B 86993-61-5
 SOL 64-17-5 EtOH

RX(2) OF 3 E ==> F



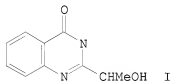
RX(2) RCT E 86993-56-8
 RGT C 75-04-7 EtNH₂
 PRO F 86993-63-7
 SOL 64-17-5 EtOH

RX(3) OF 3 G ==> H



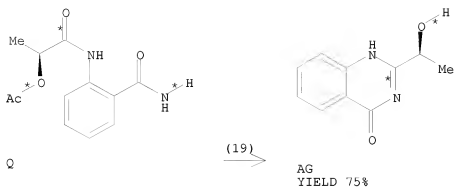
RX(3) RCT G 78993-24-5
 RGT C 75-04-7 EtNH2
 PRO H 4145-21-5
 SOL 64-17-5 EtOH

L3 ANSWER 153 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 113:171734 CASREACT
 TITLE: Synthesis of chrysogine, a metabolite of Penicillium
 chrysogenum and some related 2-substituted
 4-(3H)-quinazolinones
 AUTHOR(S): Bergman, Jan; Brynolf, Anna
 CORPORATE SOURCE: Dep. Org. Chem., R. Inst. Technol., Stockholm, S-100
 44, Swed.
 SOURCE: Tetrahedron (1990), 46(4), 1295-310
 CODEN: TETRAB; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



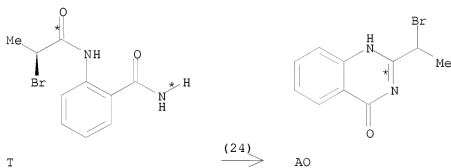
AB Both enantiomers of chrysogine (I) were prepared from 2-H2NC6H4CONH2 (II).
 Thus reaction of II and (-)-AcOCHMeCOCl gave (-)-2-AcOCHMeCONHC6H4CONH2
 which upon saponification and cyclization induced by aqueous Na2CO3 at room
 temperature gave
 (S)-(-)-I. The enantiomeric purity of (S)-(-)-I was determined by NMR.
 Inversion of (-)-(-)-I using the Mitsunobu reaction, gave (+)-(R)-I.
 Reduction of 2-acetyl-4(3H)-quinazolinone with bakers' yeast gave (S)-(-)-I.
 The cyclization method could be extended to a number of
 2-(α -hydroxy)alkyl-4-(3H)-quinazolinones.

RX(19) OF 82 ...Q ==> AG...



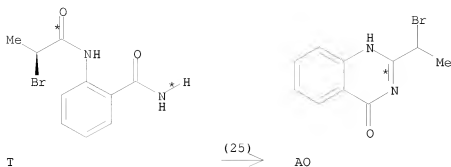
RX(19) RCT Q 129768-43-0
PRO AG 42599-89-3

RX(24) OF 82 ...T ==> AO...



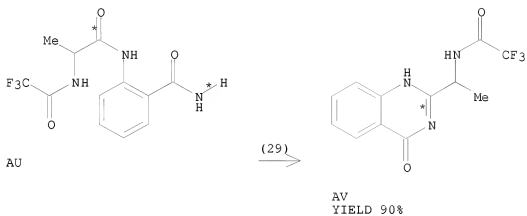
RX(24) RCT T 129831-32-9
PRO AO 144189-81-1
CAT 104-15-4 TsOH

RX(25) OF 82 T ==> AO



RX(25) RCT T 129831-32-9
 PRO AO 144189-81-1
 CAT 497-19-8 Na2CO3

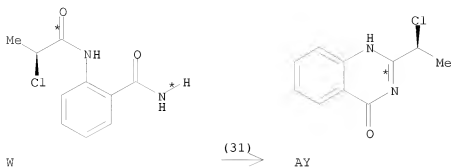
RX(29) OF 82 ...AU ==> AV



RX(29) RCT AU 129768-61-2
 PRO AV 129768-62-3

RX(31) OF 82 ...W ==> AY

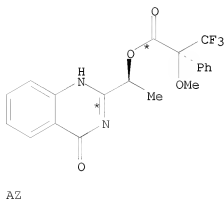
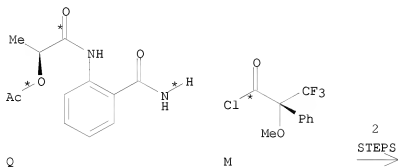
10/ 562,112



RX(31) RCT W 129768-48-5
 PRO AY 129768-63-4
 CAT 104-15-4 TsOH

RX(48) OF 82 COMPOSED OF RX(19), RX(32)

RX(48) Q + M \implies AZ

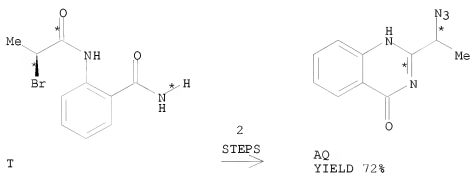


RX(19) RCT Q 129768-43-0
 PRO AG 42599-89-3

10/ 562,112

RX(32) RCT AG 42599-89-3, M 20445-33-4
 PRO AZ 151163-81-4

RX(51) OF 82 COMPOSED OF RX(24), RX(26)
 RX(51) T ==> AQ

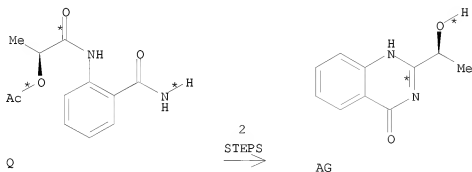


RX(24) RCT T 129831-32-9
 PRO AO 144189-81-1
 CAT 104-15-4 TsOH

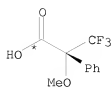
RX(26) RCT AO 144189-81-1
 RGT AR 26628-22-8 NaN₃
 PRO AQ 129768-59-8

RX(63) OF 82 COMPOSED OF REACTION SEQUENCE RX(19), RX(32)
 AND REACTION SEQUENCE RX(7), RX(32)

... Q ==> AG...
 ...L + C + AG ==> AZ



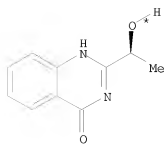
START NEXT REACTION SEQUENCE



L

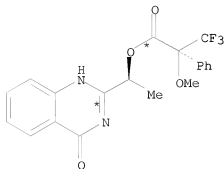


C



AG

2
STEPS
→



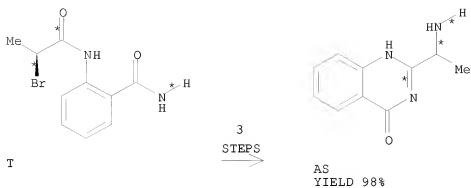
AZ

RX(19) RCT Q 129768-43-0
PRO AG 42599-89-3

RX(7) RCT L 20445-31-2, C 79-37-8
PRO M 20445-33-4

RX(32) RCT AG 42599-89-3, M 20445-33-4
PRO AZ 151163-81-4

RX(72) OF 82 COMPOSED OF RX(24), RX(26), RX(27)
RX(72) T ==> AS



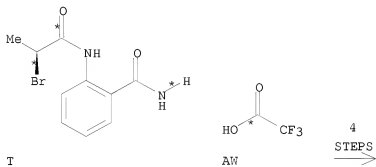
RX(24) RCT T 129831-32-9
 PRO AO 144189-81-1
 CAT 104-15-4 TsOH

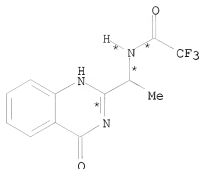
RX(26) RCT AO 144189-81-1
 RGT AR 26628-22-8 NaN₃
 PRO AQ 129768-59-8

RX(27) RCT AQ 129768-59-8
 PRO AS 172420-42-7

RX(75) OF 82 COMPOSED OF RX(24), RX(26), RX(27), RX(30)

RX(75) T + AW ==> AV

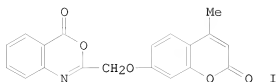




AV

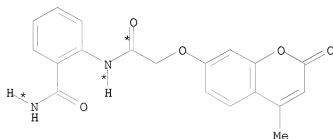
RX(24)	RCT	T 129831-32-9
	PRO	AO 144189-81-1
	CAT	104-15-4 TsOH
RX(26)	RCT	AO 144189-81-1
	RGT	AR 26628-22-8 NaN3
	PRO	AQ 129768-59-8
RX(27)	RCT	AQ 129768-59-8
	PRO	AS 172420-42-7
RX(30)	RCT	AS 172420-42-7, AW 76-05-1
	PRO	AV 129768-62-3
	CAT	144-55-8 NaHCO3

L3 ANSWER 154 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 113:78293 CASREACT
 ACCESSION NUMBER:
 TITLE: Synthesis and reactions of a
 2-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)oxomethyl-4H-
 3,1-benzoxazin-4-one
 AUTHOR(S): Soliman, A. Y.; El-Assy, N. B.; El-Shahed, F.;
 El-Kady, M.; El-Deen, I. M.
 CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
 SOURCE: Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (1990),
 29B(4), 326-30
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



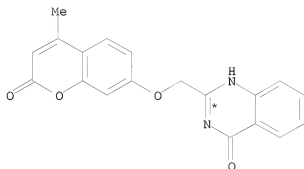
AB The relative reactivity of α -pyrone and oxazinone rings in 2-(4-methyl-2-oxo-2H-1-benzopyran-7-yloxomethyl)-4H-3,1-benzoxazin-4-one (I) towards nucleophiles (arylation under Friedel Crafts conditions, aminolysis and hydrazinolysis) and electrophiles (aromatic aldehydes) has been described.

RX(17) OF 128 ...AJ ==> AM



AJ

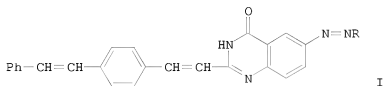
(17) \longrightarrow



AM

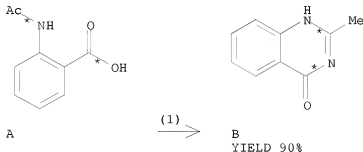
RX(17) RCT AJ 128649-83-2
 RGT AN 108-24-7 Ac20
 PRO AM 128649-84-3

L3 ANSWER 155 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 113:42449 CASREACT
 TITLE: Synthesis of azo disperse dyes from 2-(bis styryl)-6-amino-4-oxoquinazoline and their application on polyester fibers
 AUTHOR(S): Naik, N. M.; Desai, K. R.
 CORPORATE SOURCE: Dep. Chem., South Gujarat Univ., Surat, 395 007, India
 SOURCE: Indian Journal of Textile Research (1989), 14(4), 184-6
 CODEN: IJTRDU; ISSN: 0377-8436
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



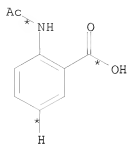
AB The title dyes (I; R = from Naphthol AS, AS-G, AS-D, AS-E, AS-BS, AS-OL, AS-BO, or AS-SW, or BON acid) were synthesized by azo coupling and color and fastness properties of I on polyester fabrics were determined

RX(1) OF 21 A ==> B...



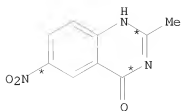
RX(1) RCT A 89-52-1
 PRO B 1769-24-0

RX(7) OF 21 COMPOSED OF RX(1), RX(2)
 RX(7) A ==> C



A

2
STEPS
→

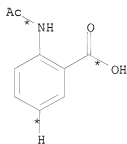


C
YIELD 95%

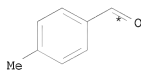
RX(1) RCT A 89-52-1
PRO B 1769-24-0

RX(2) RCT B 1769-24-0
PRO C 24688-36-6

RX(12) OF 21 COMPOSED OF RX(1), RX(2), RX(3)
RX(12) A + D ==> E

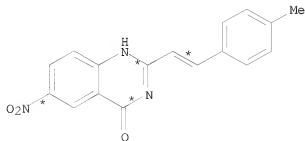


A



D

3
STEPS
→



E
YIELD 80%

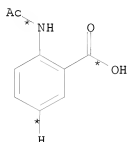
RX(1) RCT A 89-52-1
PRO B 1769-24-0

10/ 562,112

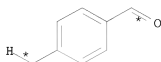
RX(2) RCT B 1769-24-0
PRO C 24688-36-6

RX(3) RCT C 24688-36-6, D 104-87-0
PRO E 73673-70-8

RX(14) OF 21 COMPOSED OF RX(1), RX(2), RX(3), RX(4)
RX(14) A + D + F ==> G



A

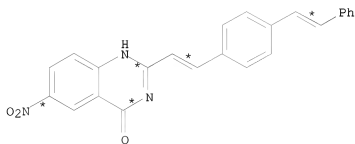


D



F

4
STEPS
→



G
YIELD 83%

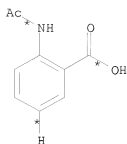
RX(1) RCT A 89-52-1
PRO B 1769-24-0

RX(2) RCT B 1769-24-0
PRO C 24688-36-6

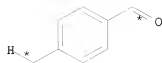
RX(3) RCT C 24688-36-6, D 104-87-0
PRO E 73673-70-8

RX(4) RCT E 73673-70-8, F 100-52-7
PRO G 128031-42-5

RX(19) OF 21 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5)
RX(19) A + D + F ==> H



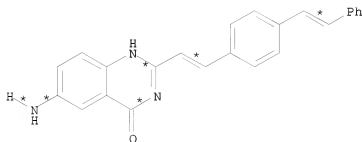
A



D



F

5
STEPS
→

H

YIELD 87%

RX(1) RCT A 89-52-1
PRO B 1769-24-0

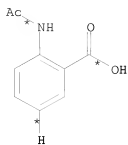
RX(2) RCT B 1769-24-0
PRO C 24688-36-6

RX(3) RCT C 24688-36-6, D 104-87-0
PRO E 73673-70-8

RX(4) RCT E 73673-70-8, F 100-52-7
PRO G 128031-42-5

RX(5) RCT G 128031-42-5
PRO H 128031-43-6

RX(21) OF 21 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6)
RX(21) A + D + F + I ==> J



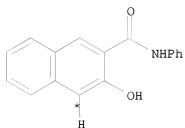
A



D

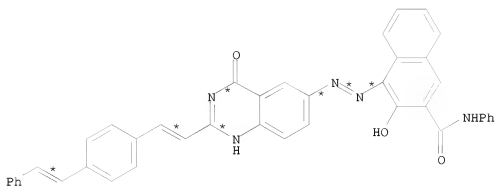


F



I

6
STEPS
→



J

YIELD 76%

RX(1) RCT A 89-52-1
PRO B 1769-24-0

RX(2) RCT B 1769-24-0
PRO C 24688-36-6

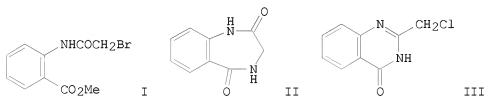
RX(3) RCT C 24688-36-6, D 104-87-0
PRO E 73673-70-8

RX(4) RCT E 73673-70-8, F 100-52-7
 PRO G 128031-42-5

RX(5) RCT G 128031-42-5
 PRO H 128031-43-6

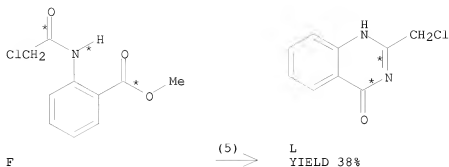
RX(6) RCT H 128031-43-6, I 92-77-3
 PRO J 128031-35-6

L3 ANSWER 156 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 113:40636 CASREACT
 TITLE: Ring closure reactions of methyl
 N-(haloacetyl)anthranilates with ammonia
 AUTHOR(S): Cho, Nam Sook; Song, Ki Youn; Parkanyi, Cyril
 CORPORATE SOURCE: Dep. Chem., Chungnam Natl. Univ., Daejeon, 302-764, S.
 Korea
 SOURCE: Journal of Heterocyclic Chemistry (1989), 26(6),
 1807-10
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



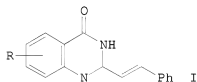
AB In the presence of ammonia, Me N-(bromoacetyl)anthranilate (I) is cyclized into 3H-1,4-benzodiazepine-2,5(1H,4H)-dione (II). However, when I is replaced with Me N-(chloroacetyl)anthranilate, the only heterocyclic product formed in the reaction is 2-(chloromethyl)quinazoline-4(3H)-one (III). Under analogous conditions, 3-haloacetamidocrotonates RCH2CONHMe:CHCO2Et (R = Br, Cl) do not yield any heterocyclic products and no 1,4-diazepines can be obtained.

RX(5) OF 11 ...F ==> L



RX(5) RCT F 58915-18-7
 RGT I 7664-41-7 NH3
 PRO L 3817-05-8
 SOL 67-56-1 MeOH

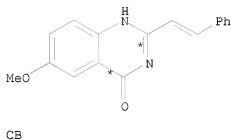
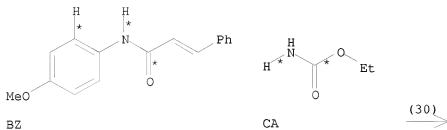
L3 ANSWER 157 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 112:235257 CASREACT
 TITLE: Synthesis and biological evaluation of
 2-styrylquinazolin-4(3H)-ones, a new class of
 antimitotic anticancer agents which inhibit tubulin
 polymerization
 AUTHOR(S): Jiang, Jack B.; Hesson, D. P.; Dusak, B. A.; Dexter,
 D. L.; Kang, G. J.; Hamel, E.
 CORPORATE SOURCE: E. I. Du Pont de Nemours and Co., Wilmington, DE,
 19880, USA
 SOURCE: Journal of Medicinal Chemistry (1990), 33(6), 1721-8
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Title compds., e.g., I (R = 5-, 6-, 7-, 8-Cl, 6-Br, 6-F, 6-NH2, 6-OMe, 5-, 6-Me, 6-OH, 6-OEt) were prepared. Extensive structure-activity relationship studies suggest that the entire quinazolinone structure was required, but activity was further enhanced by halide or small hydrophobic substituents at position 6. These analogs did not substantially interfere with the binding of radiolabeled colchicine, vinblastine, or GTP to tubulin and weakly stimulated GTP hydrolysis uncoupled from polymerization. Several analogs have shown in vivo tumor growth inhibitory activity in the L1210 leukemia model, with the lead compound I (R = 6-OMe) exhibiting good antitumor

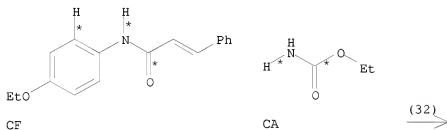
activity against murine solid tumors as well as human tumor xenografts.

RX(30) OF 64 BZ + CA ==> CB...

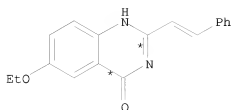


RX(30) RCT BZ 76228-15-4, CA 51-79-6
 RGT AW 1314-56-3 P205
 PRO CB 127033-41-4
 SOL 1330-20-7 Xylene

RX(32) OF 64 CF + CA ==> CG



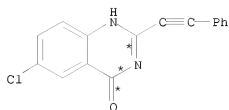
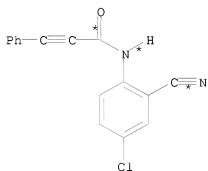
10/ 562,112



CG

RX(32) RCT CF 127033-73-2, CA 51-79-6
 RGT AW 1314-56-3 P205
 PRO CG 127033-44-7
 SOL 1330-20-7 Xylene

RX(39) OF 64 CQ ==>> CR



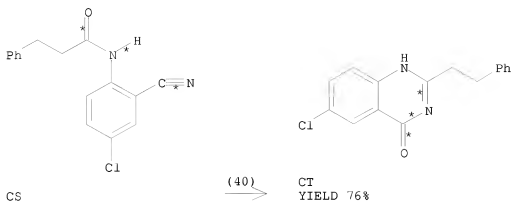
CQ



CR
YIELD 18%

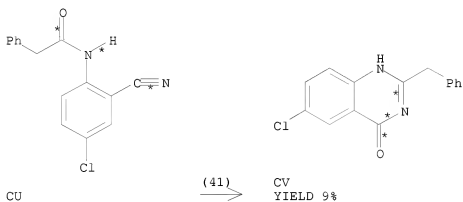
RX(39) RCT CQ 127033-75-4
 RGT E 1310-73-2 NaOH, F 7722-84-1 H2O2
 PRO CR 127033-55-0
 SOL 64-17-5 EtOH, 7732-18-5 Water

RX(40) OF 64 CS ==>> CT



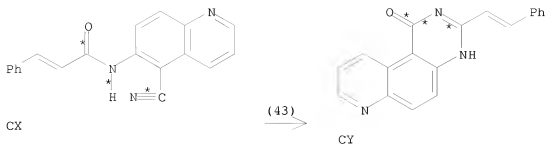
RX(40) RCT CS 127033-76-5
RGT E 1310-73-2 NaOH, F 7722-84-1 H2O2
PRO CT 127033-56-1
SOL 64-17-5 EtOH, 7732-18-5 Water

RX(41) OF 64 CU ==> CV



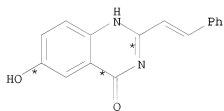
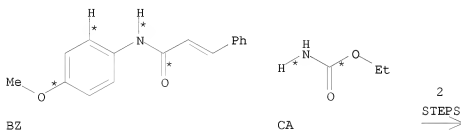
RX(41) RCT CU 127033-77-6
RGT E 1310-73-2 NaOH, F 7722-84-1 H2O2
PRO CV 35834-17-4
SOL 64-17-5 EtOH, 7732-18-5 Water

RX(43) OF 64 CX ==> CY



RX(43) RCT CX 127033-78-7
 RGT E 1310-73-2 NaOH, F 7722-84-1 H2O2
 PRO CY 127033-70-9
 SOL 64-17-5 EtOH, 7732-18-5 Water

RX(58) OF 64 COMPOSED OF RX(30), RX(31)
 RX(58) BZ + CA ==> CD



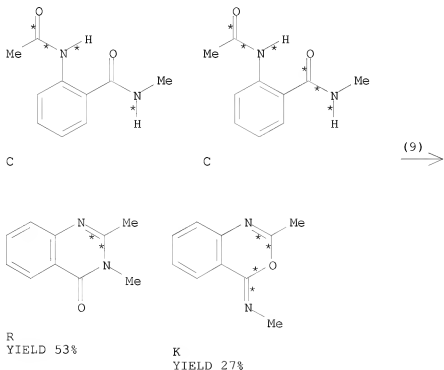
CD
 YIELD 63%

RX(30) RCT BZ 76228-15-4, CA 51-79-6
 RGT AW 1314-56-3 P205
 PRO CB 127033-41-4
 SOL 1330-20-7 Xylene

RX(31) RCT CB 127033-41-4
 RGT CE 10035-10-6 HBr
 PRO CD 127033-42-5
 SOL 7732-18-5 Water, 64-19-7 AcOH

L3 ANSWER 158 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 112:216853 CASREACT
 TITLE: Synthesis and rearrangement of
 4-imino-4H-3,1-benzoxazines
 AUTHOR(S): Mazurkiewicz, Roman
 CORPORATE SOURCE: Inst. Org. Chem. Technol., Silesian Tech. Univ.,
 Gliwice, PL-44-101, Pol.
 SOURCE: Monatshefte fuer Chemie (1989), 120(11), 973-80
 CODEN: MOCMB7; ISSN: 0026-9247
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB o-RNHOC6H4NHCOR1 (I; R, R1 = Me, Ph) react with Ph3P-Br in the presence
 of Et3N as HBr captor to give 2-methyl- or
 2-phenyl-4-imino-4H-3,1-benzoxazines in good yields. Without an acid
 acceptor, I (R1 = Me) yield 2-methyl-4-quinazolones, while I (R1 = Ph)
 give 2-phenyl-4-imino-4H-3,1-benzoxazines.
 2-Methyl-4-imino-4H-3,1-benzoxazines rearrange under the influence of HCl
 or HBr into the resp. 2-methyl-4-quinazolones; the 2-phenyl analogs,
 however, do not rearrange.

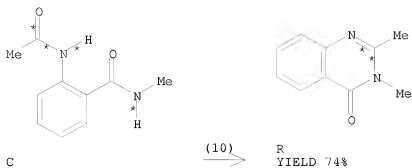
RX(9) OF 24 ...2 C ==> R + K...



RX(9) RCT C 59525-16-5
 RGT L 7726-95-6 Br2, S 7446-70-0 AlCl3
 PRO R 1769-25-1, K 127082-55-7
 SOL 75-09-2 CH2Cl2

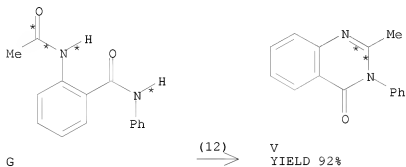
10/ 562,112

RX(10) OF 24 ...C ==> R



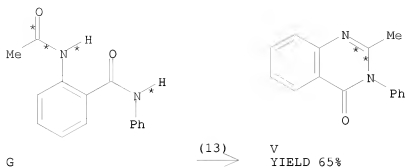
RX(10) RCT C 59525-16-5
RGT L 7726-95-6 Br2, S 7446-70-0 AlCl3
PRO R 1769-25-1
SOL 75-09-2 CH2Cl2

RX(12) OF 24 ...G ==> V



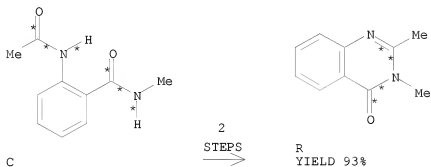
RX(12) RCT G 54364-31-7
RGT T 7647-01-0 HCl
PRO V 2385-23-1
SOL 107-06-2 ClCH2CH2Cl

RX(13) OF 24 G ==> V



RX(13) RCT G 54364-31-7
RGT L 7726-95-6 Br2, S 7446-70-0 AlCl3
PRO V 2385-23-1
SOL 75-09-2 CH2Cl2

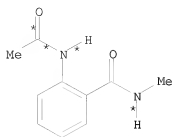
RX(21) OF 24 COMPOSED OF RX(5), RX(11)
RX(21) C ==> R



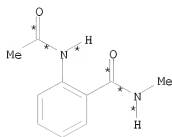
RX(5) RCT C 59525-16-5
RGT L 7726-95-6 Br2, M 603-35-0 PPh3, D 121-44-8 Et3N
PRO K 127082-55-7
SOL 75-09-2 CH2Cl2

RX(11) RCT K 127082-55-7
RGT T 7647-01-0 HCl
PRO R 1769-25-1
SOL 107-06-2 ClCH2CH2Cl

RX(22) OF 24 COMPOSED OF RX(9), RX(11)
RX(22) 2 C ==> R

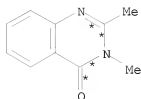


C



C

2
STEPS
→



R
YIELD 93%

RX(9) RCT C 59525-16-5
RGT L 7726-95-6 Br2, S 7446-70-0 AlCl3
PRO R 1769-25-1, K 127082-55-7
SOL 75-09-2 CH2Cl2

RX(11) RCT K 127082-55-7
RGT T 7647-01-0 HCl
PRO R 1769-25-1
SOL 107-06-2 ClCH2CH2Cl

L3 ANSWER 159 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 112:157325 CASREACT

TITLE: Dithiocarboxylic acids, dithiocarboxylic esters, or thiocarboxylic amides by reaction of methylene-active chloromethyl compounds with sulfur

AUTHOR(S): Thiel, W.; Mayer, R.

CORPORATE SOURCE: Sek. Chem., Tech. Univ. Dresden, Dresden, DDR-8027, Ger. Dem. Rep.

SOURCE: Journal fuer Praktische Chemie (Leipzig) (1989), 331(2), 243-62

CODEN: JPCEAO; ISSN: 0021-8383

DOCUMENT TYPE: Journal

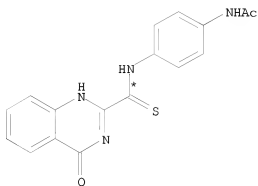
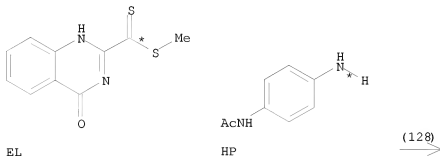
LANGUAGE: German

AB With a mixture of S and amine in DMF at room temperature halomethyl compds. can be

oxidized to give thiocarboxylic acids and their derivs. The reaction was studied in detail especially with chloroacetic derivs. or chloromethyl

heterocycles formally derived from chloroacetic acid. The resulting thiooxalic acid derivs. represent activated acids and very useful C2-synthons, especially for the synthesis of heterocycles. Oxidation in the presence of Et₃N leads to dithiocarboxylates which can be alkylated to dithioesters in high yields. As a rule, with different primary and secondary amines instead of tertiary amines these dithiocarboxylates or dithiocarboxylic esters can be transformed already at low temps. to thioamides.

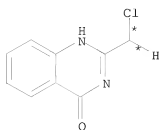
RX(128) OF 251 ...EL + HP ==> HU



HU
YIELD 75%

RX(128) RCT EL 125983-30-4, HP 122-80-5
PRO HU 125983-51-9
SOL 64-17-5 EtOH

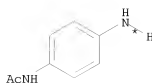
RX(247) OF 251 COMPOSED OF RX(74), RX(128)
RX(247) EK + B + HP ==> HU



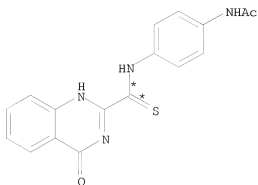
EK



B



HP

2
STEPS
→

HU

YIELD 75%

RX(74) RCT EK 3817-05-8

STAGE(1)

RGT D 7704-34-9 S, E 121-44-8 Et3N

SOL 68-12-2 DMF

STAGE(2)

RCT B 74-88-4

PRO EL 125983-30-4

RX(128) RCT EL 125983-30-4, HP 122-80-5

PRO HU 125983-51-9

SOL 64-17-5 EtOH

L3 ANSWER 160 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 112:35794 CASREACT

TITLE: Synthesis and anticonvulsant activity of some new 2-substituted 3-aryl-4(3H)-quinazolinones

AUTHOR(S): Wolfe, James F.; Rathman, Terry L.; Sleevi, Mark C.; Campbell, James A.; Greenwood, Thomas D.

CORPORATE SOURCE:

Dep. Chem., Virginia Polytech. Inst. and State Univ.,
Blacksburg, VA, 24061, USA

SOURCE:

Journal of Medicinal Chemistry (1990), 33(1), 161-6
CODEN: JMCMAR; ISSN: 0022-2623

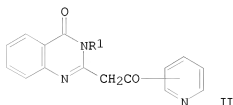
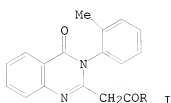
DOCUMENT TYPE:

Journal

LANGUAGE:

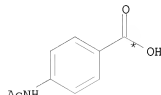
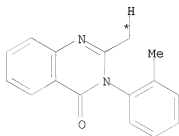
English

GI



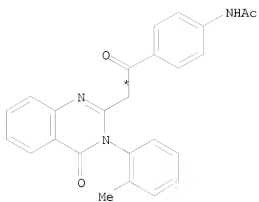
AB 4(3H)-Quinazolinones I (R = Me, Ph, 1-adamantyl, etc.) and II [R1 = (un)substituted Ph], structurally related to methaqualone were synthesized and evaluated for anticonvulsant activity. E.g., treating methaqualone with RCO2R1 (R1 = ester group) in the presence of NaH gave I. Preliminary screening of these compds. revealed that I (R = 2-pyridyl) (III) and II [o-ClC6H4 (IV), o-BrC6H4, o-FC6H4, o-MeOC6H4, o-IC6H4] having a single ortho substituent on the 3-aryl group had the most promising anticonvulsant activity. III and IV possessing 3-o-tolyl and 3-o-chlorophenyl groups, resp., showed good protection against maximum electroshock- and s.c. metrazol-induced seizures, combined with relatively low neurotoxicity after i.p. administration in mice. They also exhibited low toxicity in tests for determining the mean hypnotic dose (HD50) and the median LD (LD50). Although these compds. were markedly more potent as anticonvulsants when administered orally in mice and rats, they were also more neurotoxic. This neurotoxicity was particularly acute in oral tests with rats, which resulted in marginal protective indexes. In drug differentiation tests, III was ineffective against seizures induced by bicuculline, picrotoxin, and strychnine, while IV showed some protection against picrotoxin-induced seizures.

RX(7) OF 73 ...A + P ==> Q



esters

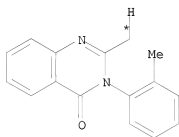




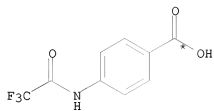
Q
YIELD 42%

RX(7) RCT A 72-44-6, P 556-08-1D
RGT D 7646-69-7 NaH
PRO Q 73283-19-9
SOL 109-99-9 THF

RX(8) OF 73 ...A + S ==> T

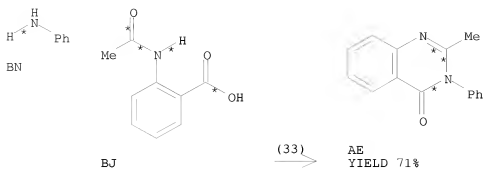


A



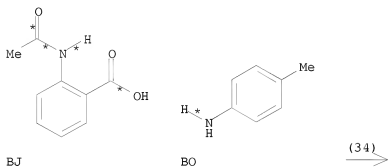
S
esters

(8) →



RX(33) RCT BN 62-53-3, BJ 89-52-1
 RGT BL 7719-12-2 PC13
 PRO AE 2385-23-1
 SOL 108-88-3 PhMe

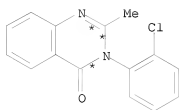
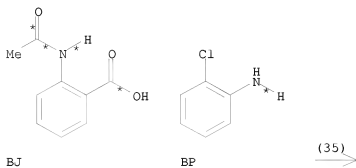
RX(34) OF 73 BJ + BO ==> AL...



AL
YIELD 77%

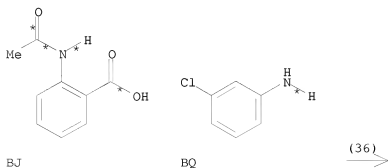
RX(34) RCT BJ 89-52-1, BO 106-49-0
 RGT BL 7719-12-2 PC13
 PRO AL 22316-59-2
 SOL 108-88-3 PhMe

RX(35) OF 73 BJ + BP ==> AP...

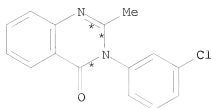
AP
YIELD 62%

RX(35) RCT BJ 89-52-1, BP 95-51-2
 RGT BL 7719-12-2 PC13
 PRO AP 340-57-8
 SOL 108-88-3 PhMe

RX(36) OF 73 BJ + BQ ==> AT...



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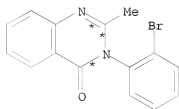
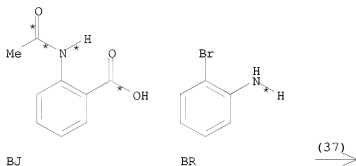


AT

YIELD 73%

RX(36) RCT BJ 89-52-1, BQ 108-42-9
RGT BL 7719-12-2 PC13
PRO AT 340-94-3
SOL 108-88-3 PhMe

RX(37) OF 73 BJ + BR ==> AV...



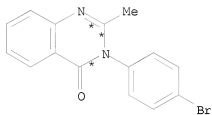
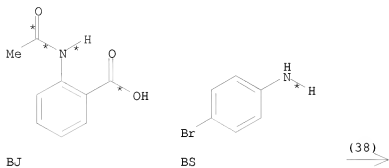
AV

YIELD 29%

RX(37) RCT BJ 89-52-1, BR 615-36-1
RGT BL 7719-12-2 PC13
PRO AV 4260-20-2
SOL 108-88-3 PhMe

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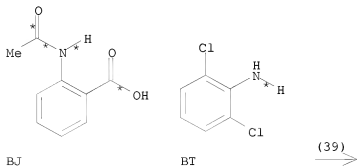
RX(38) OF 73 BJ + BS ==> AX...



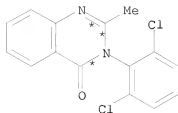
AX
YIELD 88%

RX(38) RCT BJ 89-52-1, BS 106-40-1
 RGT BL 7719-12-2 PC13
 PRO AX 1788-95-0
 SOL 108-88-3 PhMe

RX(39) OF 73 BJ + BT ==> BB...



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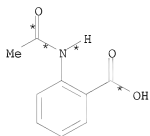


BB

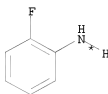
YIELD 33%

RX(39) RCT BJ 89-52-1, BT 608-31-1
 RGT BL 7719-12-2 PC13
 PRO BB 25509-06-2
 SOL 108-88-3 PhMe

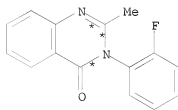
RX(40) OF 73 BJ + BU ==> BD...



BJ



BU

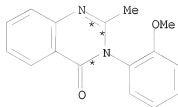
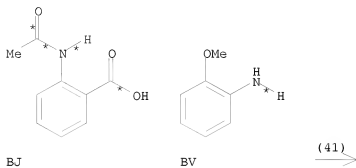


BD

YIELD 71%

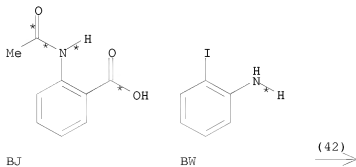
RX(40) RCT BJ 89-52-1, BU 348-54-9
 RGT BL 7719-12-2 PC13
 PRO BD 1897-87-6
 SOL 108-88-3 PhMe

RX(41) OF 73 BJ + BV ==> BF...

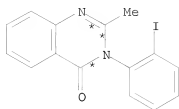
BF
YIELD 71%

RX(41) RCT BJ 89-52-1, BV 90-04-0
 RGT BL 7719-12-2 PC13
 PRO BF 4260-28-0
 SOL 108-88-3 PhMe

RX(42) OF 73 BJ + BW ==> BH...



10/ 562,112



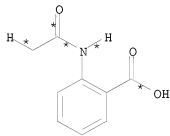
BH

YIELD 47%

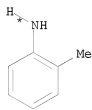
RX(42) RCT BJ 89-52-1, BW 615-43-0
 RGT BL 7719-12-2 PC13
 PRO BH 35289-03-3
 SOL 108-88-3 PhMe

RX(43) OF 73 COMPOSED OF RX(32), RX(1)

RX(43) BJ + BK + B ==> C



BJ

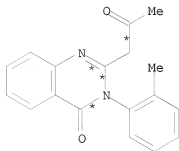


BK



B
esters

2
STEPS
→



C

YIELD 61%

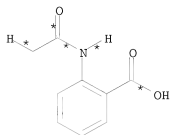
RX(32) RCT BJ 89-52-1, BK 95-53-4
 RGT BL 7719-12-2 PC13

10/ 562,112

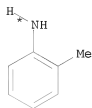
PRO A 72-44-6
SOL 108-88-3 PhMe

RX(1) RCT A 72-44-6, B 64-19-7D
RGT D 7646-69-7 NaH
PRO C 73283-07-5
SOL 110-71-4 (CH₂OMe)₂

RX(44) OF 73 COMPOSED OF RX(32), RX(2)
RX(44) BJ + BK + F ==> G



BJ

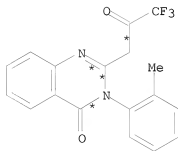


BK



F
esters

2
STEPS
→

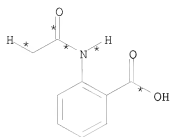


G
YIELD 87%

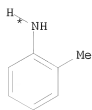
RX(32) RCT BJ 89-52-1, BK 95-53-4
RGT BL 7719-12-2 PC13
PRO A 72-44-6
SOL 108-88-3 PhMe

RX(2) RCT A 72-44-6, F 76-05-1D
RGT D 7646-69-7 NaH
PRO G 73283-08-6
SOL 110-71-4 (CH₂OMe)₂

RX(45) OF 73 COMPOSED OF RX(32), RX(3)
RX(45) BJ + BK + H ==> I



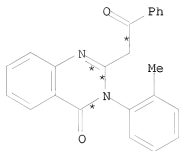
BJ



BK

H
esters

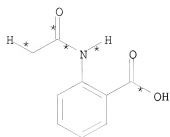
2
STEPS
→

I
YIELD 80%

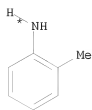
RX(32) RCT BJ 89-52-1, BK 95-53-4
RGT BL 7719-12-2 PC13
PRO A 72-44-6
SOL 108-88-3 PhMe

RX(3) RCT A 72-44-6, H 65-85-0D
RGT D 7646-69-7 NaH
PRO I 73283-14-4
SOL 110-71-4 (CH2OMe)2

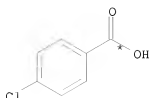
RX(46) OF 73 COMPOSED OF RX(32), RX(4)
RX(46) BJ + BK + J ==> K



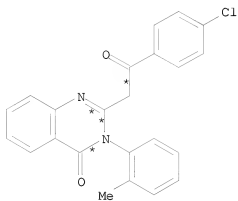
BJ



BK

J
esters

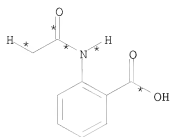
2
STEPS
→

K
YIELD 74%

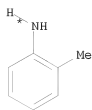
RX(32) RCT BJ 89-52-1, BK 95-53-4
RGT BL 7719-12-2 PC13
PRO A 72-44-6
SOL 108-88-3 PhMe

RX(4) RCT A 72-44-6, J 74-11-3D
RGT D 7646-69-7 NaH
PRO K 73283-15-5
SOL 110-71-4 (CH₂OMe)₂

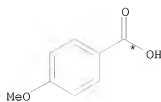
RX(47) OF 73 COMPOSED OF RX(32), RX(5)
RX(47) BJ + BK + L ==> M



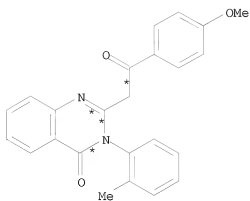
BJ



BK

L
esters

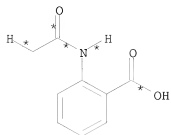
2
STEPS
→

M
YIELD 72%

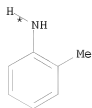
RX(32) RCT BJ 89-52-1, BK 95-53-4
 RGT BL 7719-12-2 PC13
 PRO A 72-44-6
 SOL 108-88-3 PhMe

RX(5) RCT A 72-44-6, L 100-09-4D
 RGT D 7646-69-7 NaH
 PRO M 73283-16-6
 SOL 110-71-4 (CH2OMe)2

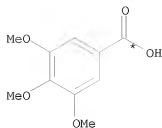
RX(48) OF 73 COMPOSED OF RX(32), RX(6)
 RX(48) BJ + BK + N ==> O



BJ

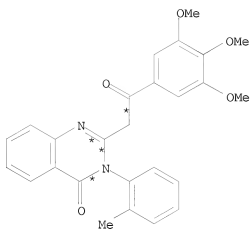


BK



N
esters

2
STEPS
→

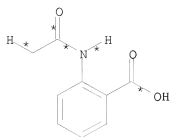


O
YIELD 67%

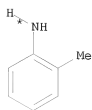
RX(32) RCT BJ 89-52-1, BK 95-53-4
 RGT BL 7719-12-2 PC13
 PRO A 72-44-6
 SOL 108-88-3 PhMe

RX(6) RCT A 72-44-6, N 118-41-2D
 RGT D 7646-69-7 NaH
 PRO O 73283-17-7
 SOL 110-71-4 (CH2OMe)2

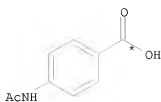
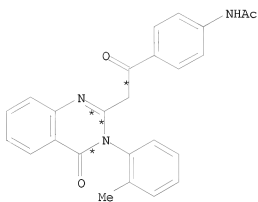
RX(49) OF 73 COMPOSED OF RX(32), RX(7)
RX(49) BJ + BK + P ==> Q



BJ



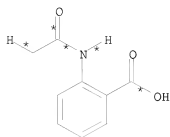
BK

P
esters2
STEPS
→Q
YIELD 42%

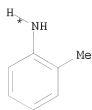
RX(32) RCT BJ 89-52-1, BK 95-53-4
 RGT BL 7719-12-2 PC13
 PRO A 72-44-6
 SOL 108-88-3 PhMe

RX(7) RCT A 72-44-6, P 556-08-1D
 RGT D 7646-69-7 NaH
 PRO Q 73283-19-9
 SOL 109-99-9 THF

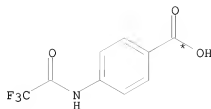
RX(50) OF 73 COMPOSED OF RX(32), RX(8)
 RX(50) BJ + BK + S ==> T



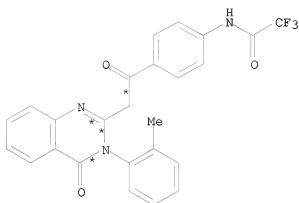
BJ



BK

S
esters

2
STEPS
→

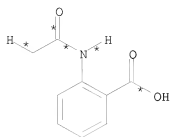


T
YIELD 47%

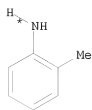
RX(32) RCT BJ 89-52-1, BK 95-53-4
RGT BL 7719-12-2 PC13
PRO A 72-44-6
SOL 108-88-3 PhMe

RX(8) RCT A 72-44-6, S 404-26-2D
RGT D 7646-69-7 NaH
PRO T 73283-18-8
SOL 109-99-9 THF

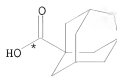
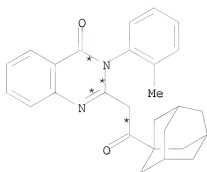
RX(51) OF 73 COMPOSED OF RX(32), RX(9)
RX(51) BJ + BK + U ==> V



BJ



BK

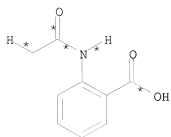
U
esters2
STEPS
→V
YIELD 81%

RX(32) RCT BJ 89-52-1, BK 95-53-4
 RGT BL 7719-12-2 PC13
 PRO A 72-44-6
 SOL 108-88-3 PhMe

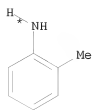
RX(9) RCT A 72-44-6, U 828-51-3D
 RGT D 7646-69-7 NaH
 PRO V 73283-12-2
 SOL 110-71-4 (CH2OMe)2

RX(52) OF 73 COMPOSED OF RX(32), RX(10)

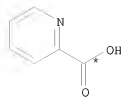
RX(52) BJ + BK + W ==> X



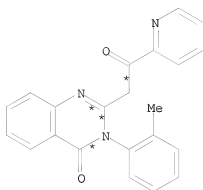
BJ



BK

W
esters

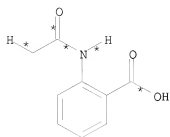
2
STEPS
→

X
YIELD 80%

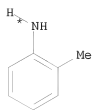
RX(32) RCT BJ 89-52-1, BK 95-53-4
RGT BL 7719-12-2 PC13
PRO A 72-44-6
SOL 108-88-3 PhMe

RX(10) RCT A 72-44-6, W 98-98-6D
RGT D 7646-69-7 NaH
PRO X 73283-09-7
SOL 110-71-4 (CH₂OMe)₂

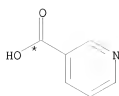
RX(53) OF 73 COMPOSED OF RX(32), RX(11)
RX(53) BJ + BK + Y ==> Z



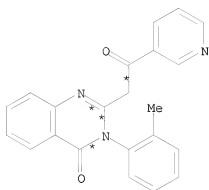
BJ



BK

Y
esters

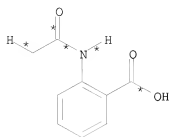
2
STEPS
→

Z
YIELD 70%

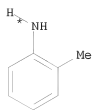
RX(32) RCT BJ 89-52-1, BK 95-53-4
RGT BL 7719-12-2 PC13
PRO A 72-44-6
SOL 108-88-3 PhMe

RX(11) RCT A 72-44-6, Y 59-67-6D
RGT D 7646-69-7 NaH
PRO Z 73283-10-0
SOL 110-71-4 (CH2OMe)2

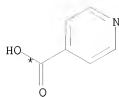
RX(54) OF 73 COMPOSED OF RX(32), RX(12)
RX(54) BJ + BK + AA ==> AB



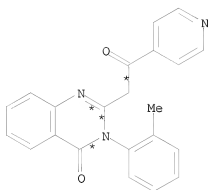
BJ



BK

AA
esters

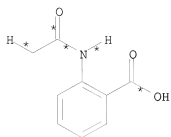
2
STEPS
→

AB
YIELD 85%

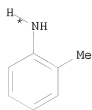
RX(32) RCT BJ 89-52-1, BK 95-53-4
RGT BL 7719-12-2 PC13
PRO A 72-44-6
SOL 108-88-3 PhMe

RX(12) RCT A 72-44-6, AA 55-22-1D
RGT D 7646-69-7 NaH
PRO AB 73283-11-1
SOL 110-71-4 (CH₂OMe)₂

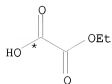
RX(55) OF 73 COMPOSED OF RX(32), RX(13)
RX(55) BJ + BK + AC ==> AD



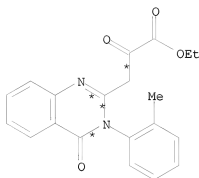
BJ



BK

AC
esters

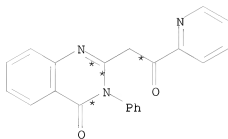
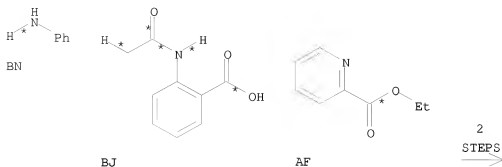
2
STEPS
➞

AD
YIELD 62%

RX(32) RCT BJ 89-52-1, BK 95-53-4
RGT BL 7719-12-2 PC13
PRO A 72-44-6
SOL 108-88-3 PhMe

RX(13) RCT A 72-44-6, AC 617-37-8D
RGT D 7646-69-7 NaH
PRO AD 56232-60-1
SOL 110-71-4 (CH2OMe)2

RX(56) OF 73 COMPOSED OF RX(33), RX(14)
RX(56) BN + BJ + AF ==> AG



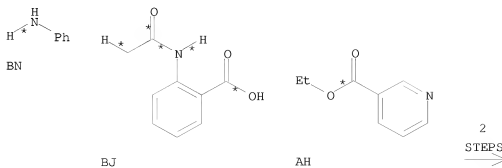
YIELD 76%

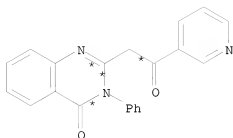
RX(33) RCT BN 62-53-3, BJ 89-52-1
RGT BL 7719-12-2 PC13
PRO AE 2385-23-1
SOL 108-88-3 PhMe

RX(14) RCT AE 2385-23-1, AF 2524-52-9
RGT D 7646-69-7 NaH
PRO AG 73283-25-7
SOL 110-71-4 (CH2OMe)2

RX(57) OF 73 COMPOSED OF RX(33), RX(15)

RX(57) BN + BJ + AH ==> AI



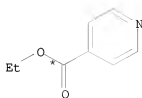
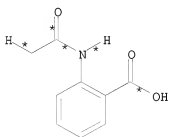


AI
YIELD 72%

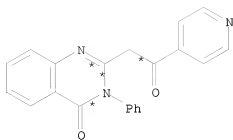
RX(33) RCT BN 62-53-3, BJ 89-52-1
RGT BL 7719-12-2 PC13
PRO AE 2385-23-1
SOL 108-88-3 PhMe

RX(15) RCT AE 2385-23-1, AH 614-18-6
RGT D 7646-69-7 NaH
PRO AI 73283-26-8
SOL 110-71-4 (CH₂OMe)₂

RX(58) OF 73 COMPOSED OF RX(33), RX(16)
RX(58) BN + BJ + AJ ==> AK



2
STEPS
=>



AK

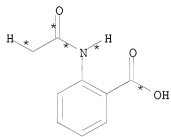
YIELD 62%

RX(33) RCT BN 62-53-3, BJ 89-52-1
 RGT BL 7719-12-2 PC13
 PRO AE 2385-23-1
 SOL 108-88-3 PhMe

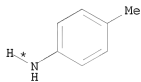
RX(16) RCT AE 2385-23-1, AJ 1570-45-2
 RGT D 7646-69-7 NaH
 PRO AK 73283-27-9
 SOL 110-71-4 (CH₂OMe)₂

RX(59) OF 73 COMPOSED OF RX(34), RX(17)

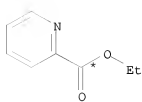
RX(59) BJ + BO + AF ==> AM



BJ

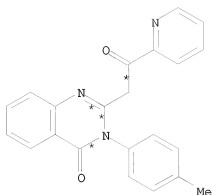


BO



AF

2
 STEPS
 →

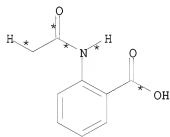


AM
YIELD 76%

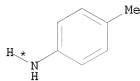
RX(34) RCT BJ 89-52-1, BO 106-49-0
RGT BL 7719-12-2 PC13
PRO AL 22316-59-2
SOL 108-88-3 PhMe

RX(17) RCT AL 22316-59-2, AF 2524-52-9
RGT D 7646-69-7 NaH
PRO AM 73283-29-1
SOL 110-71-4 (CH₂OMe)₂

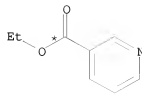
RX(60) OF 73 COMPOSED OF RX(34), RX(18)
RX(60) BJ + BO + AH ==> AN



BJ



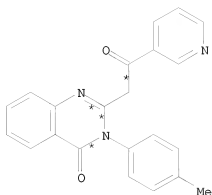
BO



AH

2
STEPS
→

10/ 562,112

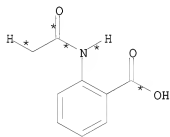


AN
YIELD 81%

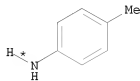
RX(34) RCT BJ 89-52-1, BO 106-49-0
 RGT BL 7719-12-2 PC13
 PRO AL 22316-59-2
 SOL 108-88-3 PhMe

RX(18) RCT AL 22316-59-2, AH 614-18-6
 RGT D 7646-69-7 NaH
 PRO AN 73283-30-4
 SOL 110-71-4 (CH₂OMe)₂

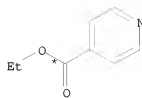
RX(61) OF 73 COMPOSED OF RX(34), RX(19)
RX(61) BJ + BO + AJ ==> AO



BJ



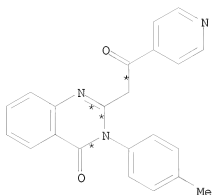
BO



AJ

2
STEPS
→

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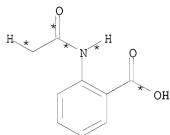


AO
YIELD 84%

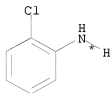
RX(34) RCT BJ 89-52-1, BO 106-49-0
 RGT BL 7719-12-2 PC13
 PRO AL 22316-59-2
 SOL 108-88-3 PhMe

RX(19) RCT AL 22316-59-2, AJ 1570-45-2
 RGT D 7646-69-7 NaH
 PRO AO 73283-31-5
 SOL 110-71-4 (CH₂OMe)₂

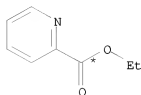
RX(62) OF 73 COMPOSED OF RX(35), RX(20)
RX(62) BJ + BP + AF ==> AQ



BJ

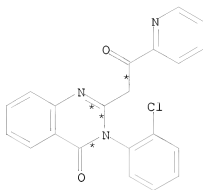


BP



AF

2
STEPS
→



AQ

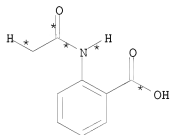
YIELD 82%

RX(35) RCT BJ 89-52-1, BP 95-51-2
 RGT BL 7719-12-2 PC13
 PRO AP 340-57-8
 SOL 108-88-3 PhMe

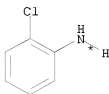
RX(20) RCT AP 340-57-8, AF 2524-52-9
 RGT D 7646-69-7 NaH
 PRO AQ 73283-21-3
 SOL 110-71-4 (CH₂OMe)₂

RX(63) OF 73 COMPOSED OF RX(35), RX(21)

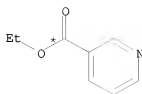
RX(63) BJ + BP + AH ==> AR



BJ

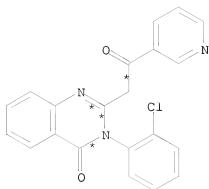


BP



AH

2
 STEPS
 ==>



AR

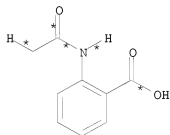
YIELD 79%

RX(35) RCT BJ 89-52-1, BP 95-51-2
RGT BL 7719-12-2 PC13
PRO AP 340-57-8
SOL 108-88-3 PhMe

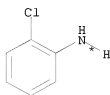
RX(21) RCT AP 340-57-8, AH 614-18-6
RGT D 7646-69-7 NaH
PRO AR 73283-22-4
SOL 110-71-4 (CH₂OMe)₂

RX(64) OF 73 COMPOSED OF RX(35), RX(22)

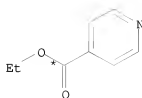
RX(64) BJ + BP + AJ ==> AS



BJ

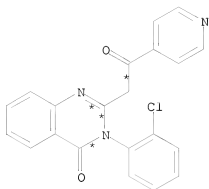


BP



AJ

2
STEPS
=>



AS

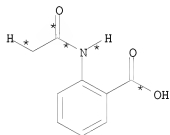
YIELD 92%

RX(35) RCT BJ 89-52-1, BP 95-51-2
 RGT BL 7719-12-2 PC13
 PRO AP 340-57-8
 SOL 108-88-3 PhMe

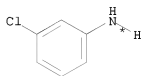
RX(22) RCT AP 340-57-8, AJ 1570-45-2
 RGT D 7646-69-7 NaH
 PRO AS 73283-23-5
 SOL 110-71-4 (CH₂OMe)₂

RX(65) OF 73 COMPOSED OF RX(36), RX(23)

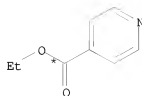
RX(65) BJ + BQ + AJ ==> AU



BJ



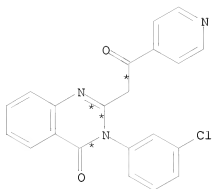
BQ



AJ

2
 STEPS
 →

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AU

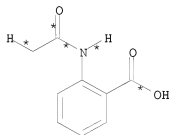
YIELD 70%

RX(36) RCT BJ 89-52-1, BQ 108-42-9
RGT BL 7719-12-2 PC13
PRO AT 340-94-3
SOL 108-88-3 PhMe

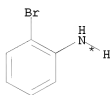
RX(23) RCT AT 340-94-3, AJ 1570-45-2
RGT D 7646-69-7 NaH
PRO AU 123382-21-8
SOL 110-71-4 (CH₂OMe)₂

RX(66) OF 73 COMPOSED OF RX(37), RX(24)

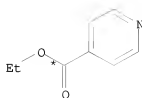
RX(66) BJ + BR + AJ ==> AW



BJ

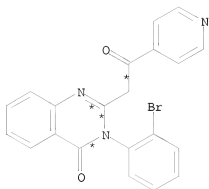


BR



AJ

2
STEPS
=>



AW

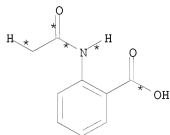
YIELD 70%

RX(37) RCT BJ 89-52-1, BR 615-36-1
RGT BL 7719-12-2 PC13
PRO AV 4260-20-2
SOL 108-88-3 PhMe

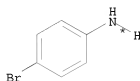
RX(24) RCT AV 4260-20-2, AJ 1570-45-2
RGT D 7646-69-7 NaH
PRO AW 123382-22-9
SOL 110-71-4 (CH₂OMe)₂

RX(67) OF 73 COMPOSED OF RX(38), RX(25)

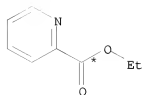
RX(67) BJ + BS + AF ==> AY



BJ

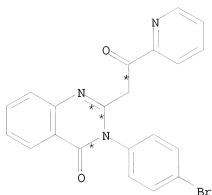


BS



AF

2
STEPS
=>

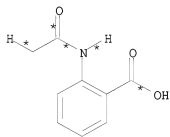


AY
YIELD 96%

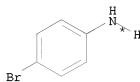
RX(38) RCT BJ 89-52-1, BS 106-40-1
RGT BL 7719-12-2 PC13
PRO AX 1788-95-0
SOL 108-88-3 PhMe

RX(25) RCT AX 1788-95-0, AF 2524-52-9
RGT D 7646-69-7 NaH
PRO AY 73283-33-7
SOL 110-71-4 (CH₂OMe)₂

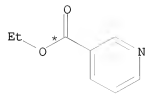
RX(68) OF 73 COMPOSED OF RX(38), RX(26)
RX(68) BJ + BS + AH ==> AZ



BJ



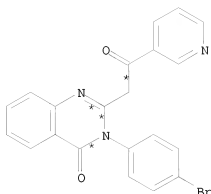
BS



AH

2
STEPS
→

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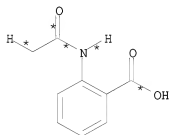


AZ
YIELD 92%

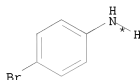
RX(38) RCT BJ 89-52-1, BS 106-40-1
 RGT BL 7719-12-2 PC13
 PRO AX 1788-95-0
 SOL 108-88-3 PhMe

RX(26) RCT AX 1788-95-0, AH 614-18-6
 RGT D 7646-69-7 NaH
 PRO AZ 73283-34-8
 SOL 110-71-4 (CH₂OMe)₂

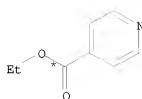
RX(69) OF 73 COMPOSED OF RX(38), RX(27)
RX(69) BJ + BS + AJ ==> BA



BJ



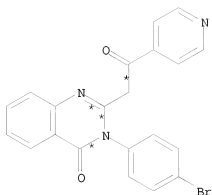
BS



AJ

2
STEPS
→

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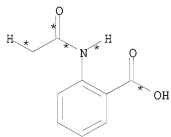


BA
YIELD 90%

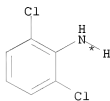
RX(38) RCT BJ 89-52-1, BS 106-40-1
 RGT BL 7719-12-2 PC13
 PRO AX 1788-95-0
 SOL 108-88-3 PhMe

RX(27) RCT AX 1788-95-0, AJ 1570-45-2
 RGT D 7646-69-7 NaH
 PRO BA 73283-35-9
 SOL 110-71-4 (CH₂OMe)₂

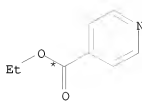
RX(70) OF 73 COMPOSED OF RX(39), RX(28)
RX(70) BJ + BT + AJ ==> BC



BJ



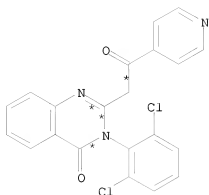
BT



AJ

2
STEPS
→

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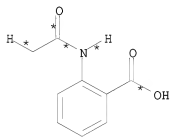


BC
YIELD 72%

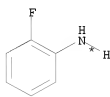
RX(39) RCT BJ 89-52-1, BT 608-31-1
 RGT BL 7719-12-2 PC13
 PRO BB 25509-06-2
 SOL 108-88-3 PhMe

RX(28) RCT BB 25509-06-2, AJ 1570-45-2
 RGT D 7646-69-7 NaH
 PRO BC 123382-23-0
 SOL 110-71-4 (CH₂OMe)₂

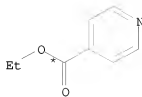
RX(71) OF 73 COMPOSED OF RX(40), RX(29)
RX(71) BJ + BU + AJ ==> BE



BJ



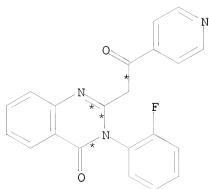
BU



AJ

2
STEPS
→

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BE

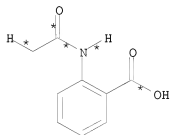
YIELD 69%

RX(40) RCT BJ 89-52-1, BU 348-54-9
 RGT BL 7719-12-2 PC13
 PRO BD 1897-87-6
 SOL 108-88-3 PhMe

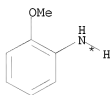
RX(29) RCT BD 1897-87-6, AJ 1570-45-2
 RGT D 7646-69-7 NaH
 PRO BE 123382-24-1
 SOL 110-71-4 (CH₂OMe)₂

RX(72) OF 73 COMPOSED OF RX(41), RX(30)

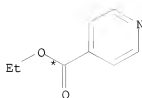
RX(72) BJ + BV + AJ ==> BG



BJ

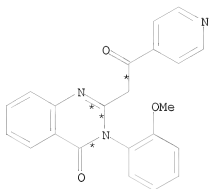


BV



AJ

2
 STEPS
 →



BG

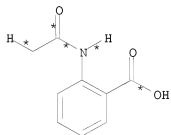
YIELD 70%

RX(41) RCT BJ 89-52-1, BV 90-04-0
 RGT BL 7719-12-2 PC13
 PRO BF 4260-28-0
 SOL 108-88-3 PhMe

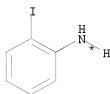
RX(30) RCT BF 4260-28-0, AJ 1570-45-2
 RGT D 7646-69-7 NaH
 PRO BG 123382-25-2
 SOL 110-71-4 (CH₂OMe)₂

RX(73) OF 73 COMPOSED OF RX(42), RX(31)

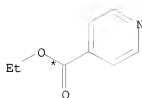
RX(73) BJ + BW + AJ ==> BI



BJ

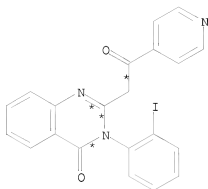


BW



AJ

2
 STEPS
 →

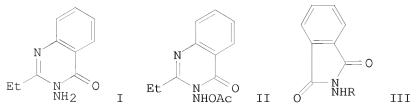


BI
YIELD 46%

RX(42) RCT BJ 89-52-1, BW 615-43-0
RGT BL 7719-12-2 PC13
PRO BH 35289-03-3
SOL 108-88-3 PhMe

RX(31) RCT BH 35289-03-3, AJ 1570-45-2
RGT D 7646-69-7 NaH
PRO BI 123382-26-3
SOL 110-71-4 (CH₂OMe)₂

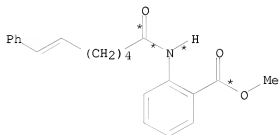
L3 ANSWER 161 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 112:35789 CASREACT
TITLE: Aziridination by oxidative addition of
N-aminoquinazolones to alkenes: evidence for
non-involvement of N-nitrenes
AUTHOR(S): Atkinson, Robert S.; Grimshire, Michael J.; Kelly,
Brian J.
CORPORATE SOURCE: Dep. Chem., Leicester Univ., Leicester, LE1 7RH, UK
SOURCE: Tetrahedron (1989), 45(10), 2875-86
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Oxidation of 3-aminoquinazolones, e.g., I, with Pb(OAc)₄ at -20° gives

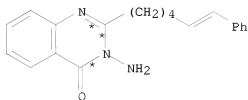
N-(acetoxyamino)quinazolones, e.g., II, which are stable in solution at this temperature. The latter compds. function as inter- and intramol. aziridinating agents for alkenes and appear to play the role previously ascribed to the corresponding N-nitrenes. An analogous N-acetoxyaminophthalimide intermediate III (R = OAc) is implicated in the Pb(OAc)₄ oxidation of III (R = H).

RX(16) OF 19 AJ ==> V...



AJ

(16) →



V

RX(16) RCT AJ 124553-59-9
 RGT AK 302-01-2 N2H4
 PRO V 124553-47-5
 SOL 64-17-5 EtOH

L3 ANSWER 162 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 112:8700 CASREACT

TITLE: Reactive disperse dyes. Synthesis of sulfonylazido group reactive disperse dyes and their application on nylon and polyester fibers

AUTHOR(S): Naik, N. M.; Desai, K. R.

CORPORATE SOURCE: Dep. Chem., South Gujarat Univ., Surat, 395 007, India

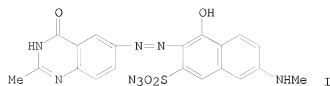
SOURCE: Journal of the Indian Chemical Society (1989), 66(7), 495-7

CODEN: JICSAH; ISSN: 0019-4522

DOCUMENT TYPE: Journal

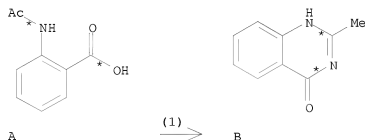
LANGUAGE: English

GI



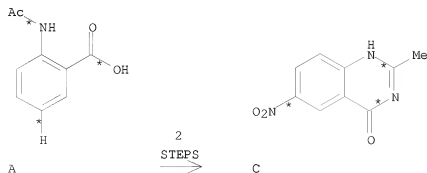
AB 2-Methyl-6-amino-4-quinazolinone was diazotized and coupled with sulfo group-containing hydroxynaphthalenes or pyrazolones and the sulfo group of the product was converted to the sulfonyl azide via the chloride. For example, I was obtained from N-Me J acid. The sulfonyl azides prepared (8) were used as reactive disperse dyes on polyamide and polyester fiber.

RX(1) OF 10 A ==> B...



RX(1) RCT A 89-52-1
PRO B 1769-24-0

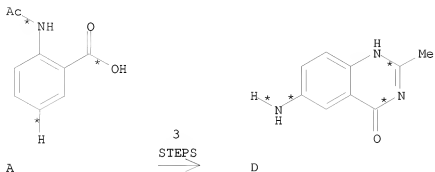
RX(5) OF 10 COMPOSED OF RX(1), RX(2)
RX(5) A ==> C



RX(1) RCT A 89-52-1
PRO B 1769-24-0

RX(2) RCT B 1769-24-0
PRO C 24688-36-6

RX(8) OF 10 COMPOSED OF RX(1), RX(2), RX(3)
 RX(8) A ==> D

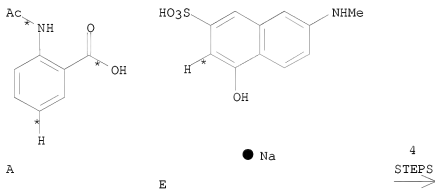


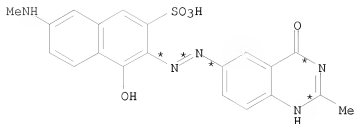
RX(1) RCT A 89-52-1
 PRO B 1769-24-0

RX(2) RCT B 1769-24-0
 PRO C 24688-36-6

RX(3) RCT C 24688-36-6
 PRO D 17329-24-7

RX(10) OF 10 COMPOSED OF RX(1), RX(2), RX(3), RX(4)
 RX(10) A + E ==> F





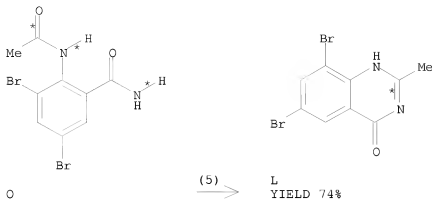
● Na

F

RX(1)	RCT A 89-52-1
	PRO B 1769-24-0
RX(2)	RCT B 1769-24-0
	PRO C 24688-36-6
RX(3)	RCT C 24688-36-6
	PRO D 17329-24-7
RX(4)	RCT D 17329-24-7, E 41494-91-1
	PRO F 124190-79-0

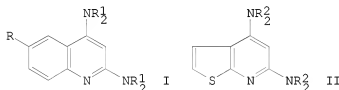
L3 ANSWER 163 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 111:194703 CASREACT
 TITLE: 6,8-Dibromo-2-methyl-1,3-4(3H)-quinazolinones
 AUTHOR(S): Ossmann, A. E.; El-Zahabi, M. M.; El-Hakim, A. E.;
 Osman, A. N.
 CORPORATE SOURCE: Org. Dep., Fac. Pharm., Cairo, Egypt
 SOURCE: Pharmazie (1989), 44(2), 113-14
 CODEN: PHARAT; ISSN: 0031-7144
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Hydrazinolysis of 6,8-dibromo-2-methyl-3,1-benzoxazin-4(H)-one afforded 3-amino-6,8-dibromo-2-methyl-1,3-4(3H)-quinazoline (I). Acylation of the latter with Ac2O and BzCl yielded the corresponding acetyl and benzoyl derivs., resp. The diazotization of I with nitrous acid led to reductive deamination and the production of 6,8-dibromo-2-methyl-1,3-4(3H)-quinazolinone.

RX(5) OF 12 ...O ==> L



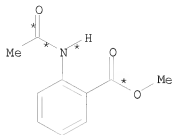
RX(5) RCT O 123434-55-9
 RGT F 108-24-7 Ac2O
 PRO L 82326-77-0

L3 ANSWER 164 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 111:153665 CASREACT
 TITLE: New one-step synthesis of
 2,4-bis(dialkylamino)quinolines and
 4,6-bis(dialkylamino)thieno[2,3-b]pyridines
 AUTHOR(S): Jensen, Jorgen A.; Pedersen, Erik B.
 CORPORATE SOURCE: Dep. Chem., Odense Univ., Odense, DK-5230, Den.
 SOURCE: Chemica Scripta (1988), 28(4), 435-7
 CODEN: CSRPB9; ISSN: 0004-2056
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB 2,4-Bis(dialkylamino)quinolines I (R = H, NR12 = morpholino, Et2N; R = H, Me, NR22 = piperidino, pyrrolidino) were prepared by heating N-acetyl-anthranilates in a mixture of P2O5, a dialkylamine hydrochloride, and N,N-dimethylcyclohexylamine at 210° for 6-10.5 h. In the same way 4,6-bis(dialkylamino)thieno[2,3-b]pyridines II (NR22 = piperidino, pyrrolidino) were prepared from Me 2-acetamido-3-thiophenecarboxylate.

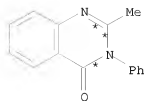
RX(2) OF 12 A + F ==> G



A

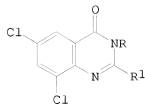


F

G
YIELD 30%

RX(2) RCT A 2719-08-6, F 100-61-8
 RGT D 1314-56-3 P205, E 98-94-2 C6H11NMe2, H 121-44-8 Et3N
 PRO G 2385-23-1

L3 ANSWER 165 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 111:130542 CASREACT
 TITLE: Synthesis and screening of some newer
 6,8-dichloro-2-methyl-3-(substituted)-4(3H)-
 quinazolinones as antimicrobial agents
 AUTHOR(S): Mohamed, Y. A.; Ammar, Y. A.; El-Sharief, A. M. S.;
 Ahmed, H.
 CORPORATE SOURCE: Fac. Sci., Al-Azhar Univ., Nasr, Egypt
 SOURCE: Proceedings of the Indian National Science Academy,
 Part A: Physical Sciences (1989), 55(1), 87-95
 CODEN: PIPSD; ISSN: 0370-0046
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



I, $R = C_6H_4SO_2NHR^2$, $R^1 = Me$

II, $R = NHCOCH_2Cl$, $R^1 = Me$

III, $R = NHCOCH_2NHR^2$, $R^1 = Me$

IV, $R = NH_2$, $R^1 = Me$

V, $R = N = CHAr$, $R^1 = Me$

VI, $R = N = CHAr$, $R^1 = CH = CHAr$

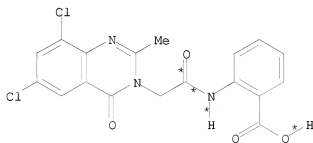
VII, $R = CH_2COC_1$, $R^1 = Me$

VIII, $R = CH_2CONHR^2$, $R^1 = Me$

IX, $R = 4\text{-oxo-2H-3,1-benzoxazinylmethyl}$, $R^1 = Me$

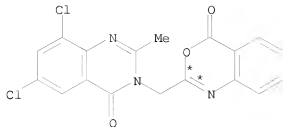
AB 6,8-Dichloro-2-methyl-3-(4-N-substituted sulfonamidophenyl)-4(3H)-quinazolinones (I, $R^2 = H$, or heterocyclic or $NHR^2 = \text{guanidino}$) were prepared by reaction of 6,8-dichloro-2-methyl-2H-3,1-benzoxazin-4-one with sulfonamides. Also, II was prepared and condensed with amines to give III ($R^2 = \text{iso-Bu}$, CH_2Ph , C_6H_4OMe-4 , or sulfonamido group). Condensation of IV with aldehydes under different conditions gave V and VI. VII underwent condensation with amines to give VIII ($R^2 = \text{aromatic or sulfonamido group}$). Cyclization of VIII ($R^2 = C_6H_4CO_2H-2$) with Ac_2O gave IX. Some of these compds. showed antimicrobial activity.

RX(37) OF 78 ...BG ==> BH



BG

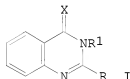
(37) →



BH

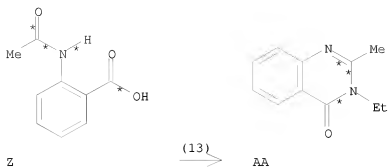
RX(37) RCT BG 122418-03-5
 PRO BH 122418-04-6
 CAT 108-24-7 Ac20

L3 ANSWER 166 OF 258 CASREACT COPYRIGHT 2009 ACS on SIN
 ACCESSION NUMBER: 111:97171 CASREACT
 TITLE: Studies on some biologically active
 azepinoquinazolines. Part I. An approach to potent
 bronchodilatory compounds
 AUTHOR(S): Malhotra, S.; Koul, S. K.; Sharma, R. L.; Anand, K.
 K.; Gupta, O. P.; Dhar, K. L.
 CORPORATE SOURCE: Nat. Prod. Chem. Div., Reg. Res. Lab., Jammu Tawi, 180
 001, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (1988),
 27B(10), 937-40
 CODEN: IJCSDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



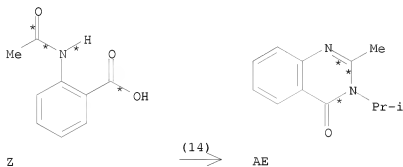
AB Quinazolines I [X = O, H₂; RR1 = (CH₂)_n; n = 3-9; R = Me, Et; R1 = CHMe₂, Pr, Bu, pentyl] have been prepared and screened for their bronchodilatory activity. I [X = O, RR1 = (CH₂)₅] has excellent bronchodilatory properties. 2,4,6-Tribromo-7,8,9,10-tetrahydroazepino[2,1-b]quinazolin 12(6H)-one, prepared by brominating I [X = O, RR1 = (CH₂)₅], shows marked antitussive and mucolytic activities parallel to those of bromhexine.

RX(13) OF 25 Z ==> AA



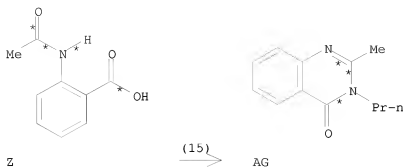
RX(13) RCT Z 89-52-1
 RGT AB 75-04-7 EtNH2
 PRO AA 50677-59-3
 CAT 110-86-1 Pyridine
 SOL 71-43-2 Benzene

RX(14) OF 25 Z ==> AE



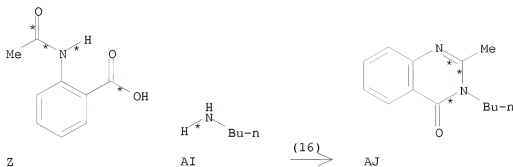
RX(14) RCT Z 89-52-1
 RGT AE 75-31-0 i-PrNH2
 PRO AE 10367-29-0
 CAT 110-86-1 Pyridine
 SOL 71-43-2 Benzene

RX(15) OF 25 Z ==> AG



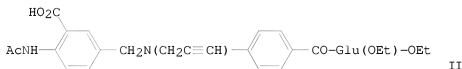
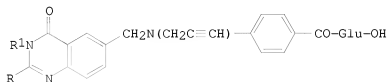
RX(15) RCT Z 89-52-1
 RGT AH 107-10-8 PrNH2
 PRO AG 50677-60-6
 CAT 110-86-1 Pyridine
 SOL 71-43-2 Benzene

RX(16) OF 25 Z + AI ==> AJ



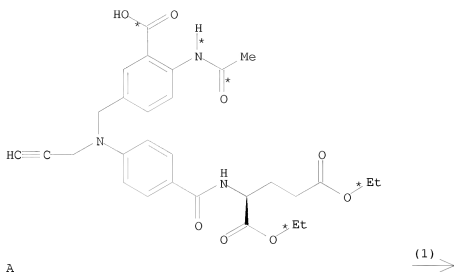
RX(16) RCT Z 89-52-1, AI 109-73-9
 RGT AC 110-86-1 Pyridine
 PRO AJ 394-90-1
 SOL 71-43-2 Benzene

L3 ANSWER 167 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 110:232041 CASREACT
 TITLE: Folate analogs. 32. Synthesis and biological
 evaluation of 2-desamino-2-methyl-N10-propargyl-5,8-
 dideazafolic acid and related compounds
 AUTHOR(S): Patil, Sharadbala D.; Jones, Cecil; Nair, M. G.;
 Galivan, J.; Maley, F.; Kisliuk, R. L.; Gaumont, Y;
 Duch, David; Ferone, Robert
 CORPORATE SOURCE: Dep. Biochem., Univ. South Alabama, Mobile, AL, 36688,
 USA
 SOURCE: Journal of Medicinal Chemistry (1989), 32(6), 1284-9



AB The chemical synthesis of 3 close analogs I (R = Me, R1 = H, Me; R = CF3, R1 = H) of N10-propargyl-5,8-dideazafolate (I, R = NH2, R1 = H) (II) is described. The quinazoline ring of I (R = Me, R1 = H, Me) was constructed from the pivotal intermediate II in a novel and unambiguous manner during the final step of the synthesis under very mild conditions. I (R = Me, R1 = H) (III) was a strong inhibitor of human and *Lactobacillus casei* thymidylate synthases, whereas I (R = R1 = Me; R = CF3, R1 = H) were only weak inhibitors of this enzyme. III exhibited excellent growth inhibition of Manca human lymphoid leukemia and H35 hepatoma cells in culture. The inhibitory activities of III were 43 and 65-fold greater than that of II, resp., in these cell lines. H35R cells that are resistant to methotrexate (MTX) by virtue of a transport defect were cross-resistant to III but not to II. H35FF cells which have 70-fold greater amts. of thymidylate synthase compared to H35N cells were 130-fold resistant to III. Furthermore, the toxicity of III to H35 hepatoma cells could be completely reversed by thymidine, establishing its locus of action as thymidylate synthase. Transport studies in vitro established that III effectively inhibits MTX influx into H35 hepatoma cells, whereas II has no effect on MTX transport in this cell line. These data suggest that the greater activity of III relative to II is partly due to the ability of the former compound to enter cells via the MTX/reduced folate transport system.

RX(1) OF 38 ...A ==> B



B
YIELD 46%

RX(1) RCT A 119820-58-5

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO₂Bu-i
SOL 68-12-2 DMF

STAGE(2)

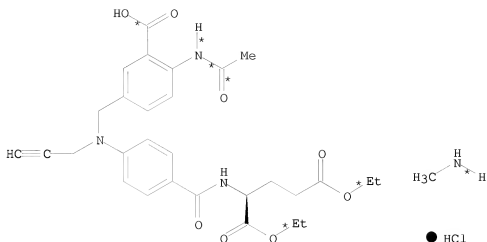
RGT E 7664-41-7 NH₃
SOL 68-12-2 DMF

STAGE(3)

RGT F 1310-73-2 NaOH
SOL 7732-18-5 Water, 75-05-8 MeCN

PRO B 112887-62-4

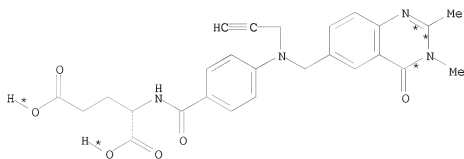
RX(3) OF 38 ...A + M ==> N



A

M

(3) →



N
YIELD 24%

RX(3) RCT A 119820-58-5

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO₂Bu-i
SOL 68-12-2 DMF

STAGE(2)

RGT M 593-51-1
RGT O 121-44-8 Et₃N
SOL 68-12-2 DMF

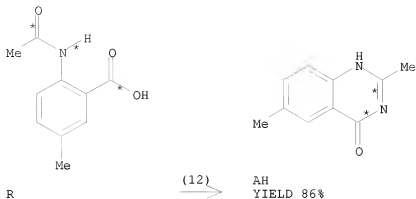
STAGE(3)

RGT F 1310-73-2 NaOH
SOL 7732-18-5 Water, 75-05-8 MeCN

PRO N 119820-56-3

RX(12) OF 38 ...R ==> AH...

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RX(12) RCT R 67081-68-9

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO₂Bu-i
SOL 68-12-2 DMF

STAGE(2)

RGT E 7664-41-7 NH₃
SOL 68-12-2 DMF

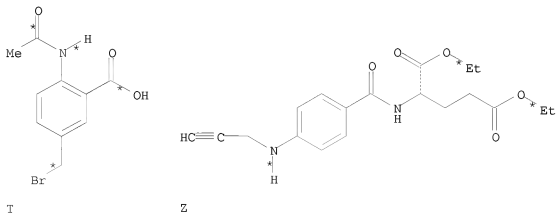
STAGE(3)

RGT F 1310-73-2 NaOH
SOL 7732-18-5 Water, 75-05-8 MeCN

PRO AH 18731-19-6

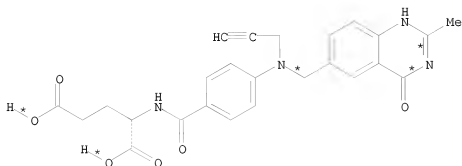
RX(17) OF 38 COMPOSED OF RX(7), RX(1)

RX(17) T + Z ==> B



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2
STEPS
→



B
YIELD 46%

RX(7) RCT T 119820-57-4, Z 76858-72-5
RGT AA 1309-48-4 MgO
PRO A 119820-58-5
SOL 127-19-5 AcNMe2

RX(1) RCT A 119820-58-5

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO2Bu-i
SOL 68-12-2 DMF

STAGE(2)

RGT E 7664-41-7 NH3
SOL 68-12-2 DMF

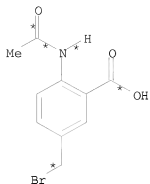
STAGE(3)

RGT F 1310-73-2 NaOH
SOL 7732-18-5 Water, 75-05-8 MeCN

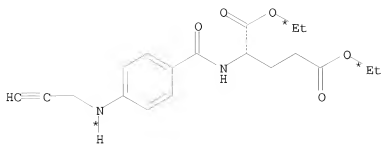
PRO B 112887-62-4

RX(18) OF 38 COMPOSED OF RX(7), RX(3)
RX(18) T + Z + M ==> N

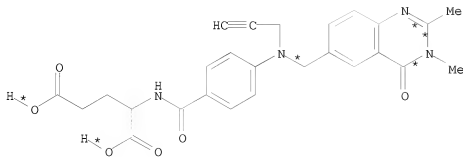
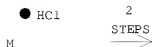
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T



Z



N

YIELD 24%

RX(7) RCT T 119820-57-4, Z 76858-72-5
RGT AA 1309-48-4 MgO
PRO A 119820-58-5
SOL 127-19-5 AcNMe2

RX(3) RCT A 119820-58-5

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClC02Bu-i
SOL 68-12-2 DMF

STAGE(2)

RCT M 593-51-1
 RGT O 121-44-8 Et3N
 SOL 68-12-2 DMF

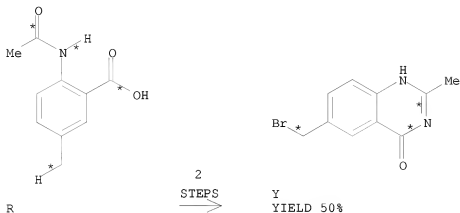
STAGE(3)

RGT F 1310-73-2 NaOH
 SOL 7732-18-5 Water, 75-05-8 MeCN

PRO N 119820-56-3

RX(23) OF 38 COMPOSED OF RX(12), RX(13)

RX(23) R ==> Y



RX(12) RCT R 67081-68-9

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO2Bu-i
 SOL 68-12-2 DMF

STAGE(2)

RGT E 7664-41-7 NH3
 SOL 68-12-2 DMF

STAGE(3)

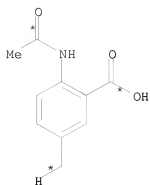
RGT F 1310-73-2 NaOH
 SOL 7732-18-5 Water, 75-05-8 MeCN

PRO AH 18731-19-6

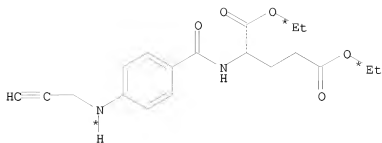
RX(13) RCT AH 18731-19-6
 RGT U 77-48-5 Br2-Me2-hydantoin
 PRO Y 112888-43-4
 CAT 94-36-0 Benzoyl peroxide
 SOL 56-23-5 CCl4, 67-66-3 CHCl3
 NTE Photochem.

RX(27) OF 38 COMPOSED OF RX(5), RX(7), RX(1)

RX(27) R + Z ==> B

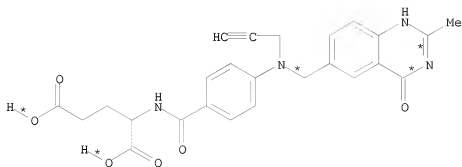


R



Z

3
STEPS
→



B

YIELD 46%

RX(5) RCT R 67081-68-9
RGT U 77-48-5 Br2-Me2-hydantoin
PRO T 119820-57-4
CAT 94-36-0 Benzoyl peroxide
SOL 67-66-3 CHCl3, 56-23-5 CCl4
NTE Photochem.

RX(7) RCT T 119820-57-4, Z 76858-72-5
RGT AA 1309-48-4 MgO
PRO A 119820-58-5
SOL 127-19-5 AcNMe2

RX(1) RCT A 119820-58-5

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO2Bu-i

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SOL 68-12-2 DMF

STAGE(2)

RGT E 7664-41-7 NH3

SOL 68-12-2 DMF

STAGE(3)

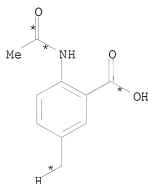
RGT F 1310-73-2 NaOH

SOL 7732-18-5 Water, 75-05-8 MeCN

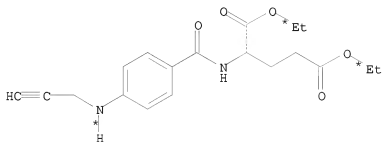
PRO B 112887-62-4

RX(28) OF 38 COMPOSED OF RX(5), RX(7), RX(3)

RX(28) R + Z + M ==> N



R



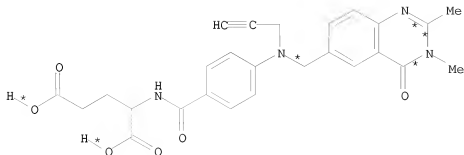
Z



M

● HCl

3
STEPS
→



N
YIELD 24%

RX(5) RCT R 67081-68-9
RGT U 77-48-5 Br2-Me2-hydantoin
PRO T 119820-57-4
CAT 94-36-0 Benzoyl peroxide
SOL 67-66-3 CHCl3, 56-23-5 CC14
NTE Photochem.

RX(7) RCT T 119820-57-4, Z 76858-72-5
RGT AA 1309-48-4 MgO
PRO A 119820-58-5
SOL 127-19-5 AcNMe2

RX(3) RCT A 119820-58-5

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClCO2Bu-i
SOL 68-12-2 DMF

STAGE(2)

RCT M 593-51-1
RGT O 121-44-8 Et3N
SOL 68-12-2 DMF

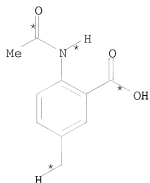
STAGE(3)

RGT F 1310-73-2 NaOH
SOL 7732-18-5 Water, 75-05-8 MeCN

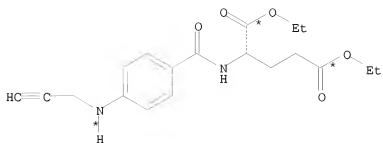
PRO N 119820-56-3

RX(36) OF 38 COMPOSED OF RX(12), RX(13), RX(6)
RX(36) R + Z ==> B

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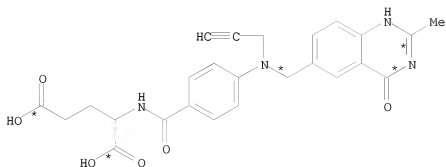


R



Z

3
STEPS
→



B

YIELD 67%

RX(12) RCT R 67081-68-9

STAGE(1)

RGT C 109-02-4 N-Methylmorpholine, D 543-27-1 ClC02Bu-i

SOL 68-12-2 DMF

STAGE(2)

RGT E 7664-41-7 NH3

SOL 68-12-2 DMF

STAGE(3)

RGT F 1310-73-2 NaOH

SOL 7732-18-5 Water, 75-05-8 MeCN

PRO AH 18731-19-6

RX(13) RCT AH 18731-19-6

RGT U 77-48-5 Br2-Me2-hydantoin
 PRO Y 112888-43-4
 CAT 94-36-0 Benzoyl peroxide
 SOL 56-23-5 CC14, 67-66-3 CHCl3
 NTE Photochem.

RX(6) RCT Y 112888-43-4, Z 76858-72-5

STAGE(1)

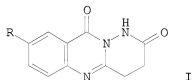
RGT AA 1309-48-4 MgO
 SOL 127-19-5 AcNMe2

STAGE(2)

RGT F 1310-73-2 NaOH
 SOL 7732-18-5 Water, 75-05-8 MeCN

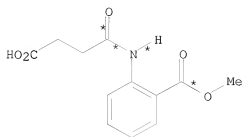
PRO B 112887-62-4

L3 ANSWER 168 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 110:212758 CASREACT
 TITLE: Reactions of cyclic anhydrides. Part XIII. Facile
 synthesis of 1,2,3,4-tetrahydro-10H-pyridazino[6,1-
 b]quinazoline-2,10-diones
 AUTHOR(S): Balasubramanian, V.; Argade, N. P.
 CORPORATE SOURCE: Sci. Res. cent., HPT Arts RYK Sci. Coll., Nashik, 422
 005, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (1988),
 27B(10), 906-8
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



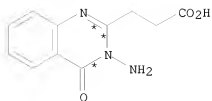
AB Pyridazinoquinazolin-2(1H)-ones I (R = H, B) have been prepared by hydrazinolysis of 4,2-R(R1O2C)C6H3NHC(=O)CH2CH2CO2R2 (R1 = Me, Et, R2 = H, Me, Et) or alkyl β-(4-oxo-3,1-benzoxazin-2-yl)propionates via alkyl β-(3-amino-4-oxoquinazolin-2-yl)propionates or β-(3-amino-4-oxoquinazolin-2-yl)propionic hydrazide. I (R = H) has also been obtained by refluxing 2-H2NC6H4CONHNH2 and succinic anhydride in dry xylene.

RX(18) OF 137 ...P ==> AF...



P

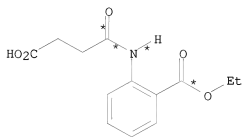
(18)
→



AF

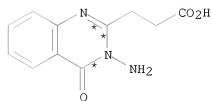
RX(18) RCT P 108540-96-1
 RGT AG 302-01-2 N2H4
 PRO AF 84312-90-3
 SOL 64-17-5 EtOH

RX(19) OF 137 ...R ==> AF...



R

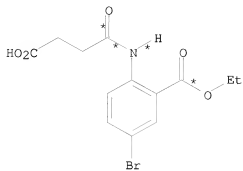
(19)
→



AF

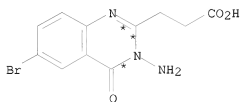
RX(19) RCT R 120572-38-5
 RGT AG 302-01-2 N2H4
 PRO AF 84312-90-3
 SOL 64-17-5 EtOH

RX(20) OF 137 ...V ==> AH...



V

(20)

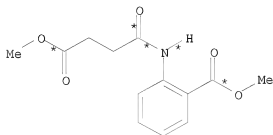


AH

YIELD 90%

RX(20) RCT V 120572-40-9
 RGT AG 302-01-2 N2H4
 PRO AH 120572-47-6
 SOL 64-17-5 EtOH

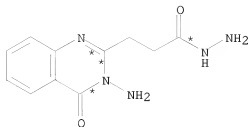
RX(24) OF 137 ...W ==> AL...



W

(24)

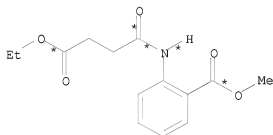
10/ 562,112



AL

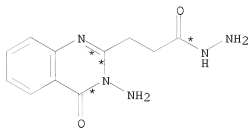
RX(24) RCT W 59868-50-7
 RGT AG 302-01-2 N2H4
 PRO AL 120572-51-2
 SOL 64-17-5 EtOH

RX(25) OF 137 ...X ==> AL...



X

(25)

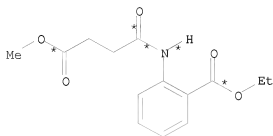


AL

RX(25) RCT X 120572-41-0
 RGT AG 302-01-2 N2H4
 PRO AL 120572-51-2
 SOL 64-17-5 EtOH

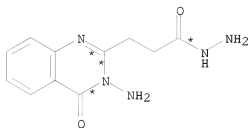
10/ 562,112

RX(26) OF 137 ...Y ==> AL...



Y

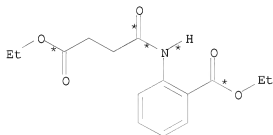
(26) →



AL

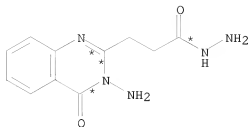
RX(26) RCT Y 120572-42-1
RGT AG 302-01-2 N2H4
PRO AL 120572-51-2
SOL 64-17-5 EtOH

RX(27) OF 137 ...Z ==> AL...



Z

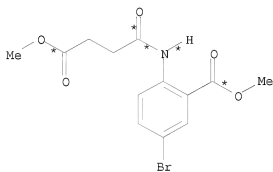
(27) →



AL

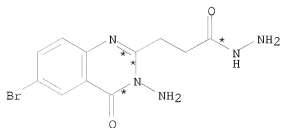
RX(27) RCT Z 120572-43-2
 RGT AG 302-01-2 N2H4
 PRO AL 120572-51-2
 SOL 64-17-5 EtOH

RX(32) OF 137 ...AA ==> AM



AA

(32) \longrightarrow

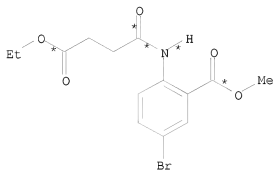


AM

RX(32) RCT AA 120572-44-3
 RGT AG 302-01-2 N2H4
 PRO AM 120572-52-3
 SOL 64-17-5 EtOH

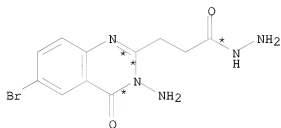
10/ 562,112

RX(33) OF 137 ...AB ==> AM



AB

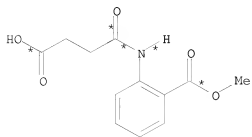
(33)



AM

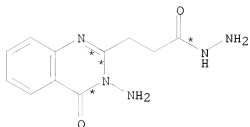
RX(33) RCT AB 120572-45-4
RGT AG 302-01-2 N2H4
PRO AM 120572-52-3
SOL 64-17-5 EtOH

RX(53) OF 137 COMPOSED OF RX(10), RX(24)
RX(53) P ==> AL



P

2
STEPS

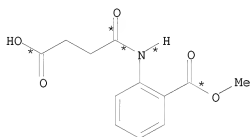


AL

RX(10) RCT P 108540-96-1
 RGT J 67-56-1 MeOH
 PRO W 59868-50-7
 CAT 7664-93-9 H2SO4
 SOL 67-56-1 MeOH

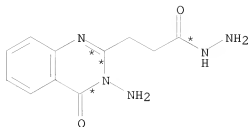
RX(24) RCT W 59868-50-7
 RGT AG 302-01-2 N2H4
 PRO AL 120572-51-2
 SOL 64-17-5 EtOH

RX(54) OF 137 COMPOSED OF RX(11), RX(25)
 RX(54) P ==> AL



P

2
 STEPS
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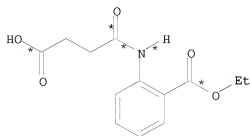
AL

RX(11) RCT P 108540-96-1
 RGT M 64-17-5 EtOH
 PRO X 120572-41-0
 CAT 7664-93-9 H2SO4
 SOL 64-17-5 EtOH

RX(25) RCT X 120572-41-0
 RGT AG 302-01-2 N2H4
 PRO AL 120572-51-2
 SOL 64-17-5 EtOH

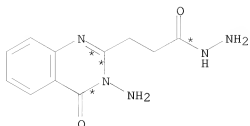
RX(55) OF 137 COMPOSED OF RX(12), RX(26)

RX(55) R ==> AL



R

2
 STEPS
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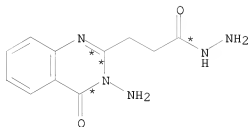
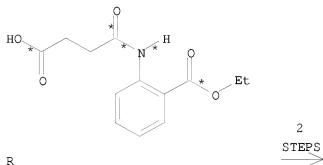
AL

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RX(12) RCT R 120572-38-5
RGT J 67-56-1 MeOH
PRO Y 120572-42-1
CAT 7664-93-9 H2SO4
SOL 67-56-1 MeOH

RX(26) RCT Y 120572-42-1
RGT AG 302-01-2 N2H4
PRO AL 120572-51-2
SOL 64-17-5 EtOH

RX(56) OF 137 COMPOSED OF RX(13), RX(27)
RX(56) R ==> AL



AL

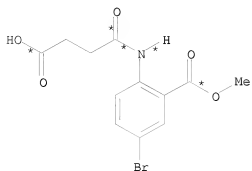
RX(13) RCT R 120572-38-5
RGT M 64-17-5 EtOH
PRO Z 120572-43-2
CAT 7664-93-9 H2SO4
SOL 64-17-5 EtOH

RX(27) RCT Z 120572-43-2
RGT AG 302-01-2 N2H4
PRO AL 120572-51-2
SOL 64-17-5 EtOH

RX(57) OF 137 COMPOSED OF RX(14), RX(32)

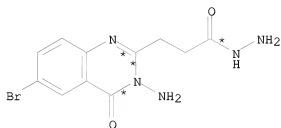
10/ 562,112

RX(57) T ==> AM



T

2
STEPS
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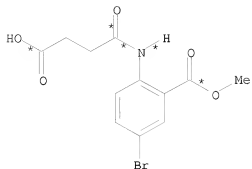


AM

RX(14) RCT T 120572-39-6
RGT J 67-56-1 MeOH
PRO AA 120572-44-3
CAT 7664-93-9 H₂SO₄
SOL 67-56-1 MeOH

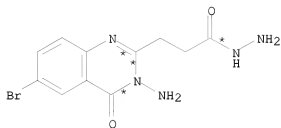
RX(32) RCT AA 120572-44-3
RGT AG 302-01-2 N₂H₄
PRO AM 120572-52-3
SOL 64-17-5 EtOH

RX(58) OF 137 COMPOSED OF RX(15), RX(33)
RX(58) T ==> AM



T

2
STEPS
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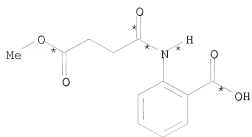
AM

RX(15) RCT T 120572-39-6
RGT M 64-17-5 EtOH
PRO AB 120572-45-4
CAT 7664-93-9 H2SO4
SOL 64-17-5 EtOH

RX(33) RCT AB 120572-45-4
RGT AG 302-01-2 N2H4
PRO AM 120572-52-3
SOL 64-17-5 EtOH

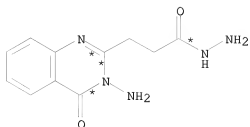
RX(59) OF 137 COMPOSED OF RX(16), RX(28)
RX(59) I ==> AL

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I

2
STEPS
→

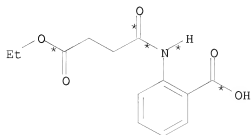


AL

RX(16) RCT I 54559-37-4
RGT AD 108-24-7 Ac2O
PRO AC 54559-36-3

RX(28) RCT AC 54559-36-3
RGT AG 302-01-2 N2H4
PRO AL 120572-51-2
SOL 64-17-5 EtOH

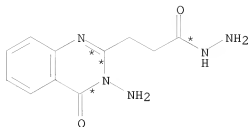
RX(60) OF 137 COMPOSED OF RX(17), RX(29)
RX(60) L ==> AL



L

2
STEPS
→

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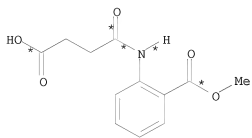


AL

RX(17) RCT L 120572-36-3
RGT AD 108-24-7 Ac2O
PRO AE 120572-46-5

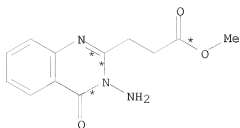
RX(29) RCT AE 120572-46-5
RGT AG 302-01-2 N2H4
PRO AL 120572-51-2
SOL 64-17-5 EtOH

RX(61) OF 137 COMPOSED OF RX(18), RX(21)
RX(61) P ==> AI



P

2
STEPS
→



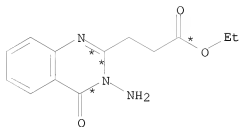
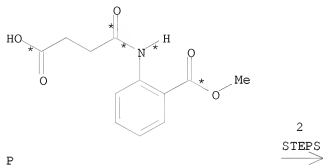
AI
YIELD 80%

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RX(18) RCT P 108540-96-1
RGT AG 302-01-2 N2H4
PRO AF 84312-90-3
SOL 64-17-5 EtOH

RX(21) RCT AF 84312-90-3
RGT J 67-56-1 MeOH
PRO AI 120572-48-7
CAT 7664-93-9 H2SO4
SOL 67-56-1 MeOH

RX(62) OF 137 COMPOSED OF RX(18), RX(22)
RX(62) P ==> AJ



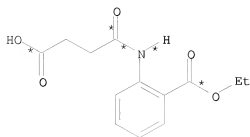
AJ
YIELD 80%

RX(18) RCT P 108540-96-1
RGT AG 302-01-2 N2H4
PRO AF 84312-90-3
SOL 64-17-5 EtOH

RX(22) RCT AF 84312-90-3
RGT M 64-17-5 EtOH
PRO AJ 120572-49-8
CAT 7664-93-9 H2SO4
SOL 64-17-5 EtOH

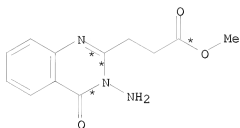
RX(63) OF 137 COMPOSED OF RX(19), RX(21)
RX(63) R ==> AI

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R

2
STEPS
→



AI

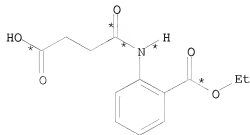
YIELD 80%

RX(19) RCT R 120572-38-5
RGT AG 302-01-2 N2H4
PRO AF 84312-90-3
SOL 64-17-5 EtOH

RX(21) RCT AF 84312-90-3
RGT J 67-56-1 MeOH
PRO AI 120572-48-7
CAT 7664-93-9 H2SO4
SOL 67-56-1 MeOH

RX(64) OF 137 COMPOSED OF RX(19), RX(22)

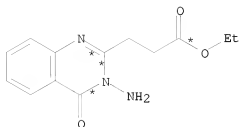
RX(64) R ==> AJ



R

2
STEPS
→

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AJ

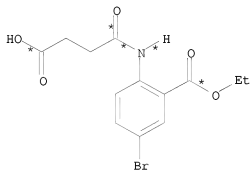
YIELD 80%

RX(19) RCT R 120572-38-5
 RGT AG 302-01-2 N2H4
 PRO AF 84312-90-3
 SOL 64-17-5 EtOH

RX(22) RCT AF 84312-90-3
 RGT M 64-17-5 EtOH
 PRO AJ 120572-49-8
 CAT 7664-93-9 H2SO4
 SOL 64-17-5 EtOH

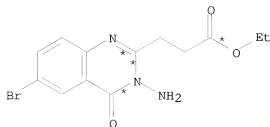
RX(65) OF 137 COMPOSED OF RX(20), RX(23)

RX(65) V ==> AK



V

2
STEPS
→



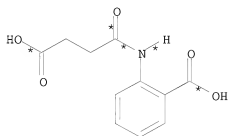
AK

YIELD 85%

RX(20) RCT V 120572-40-9
 RGT AG 302-01-2 N2H4
 PRO AH 120572-47-6
 SOL 64-17-5 EtOH

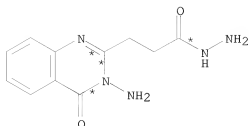
RX(23) RCT AH 120572-47-6
 RGT M 64-17-5 EtOH
 PRO AK 120572-50-1
 CAT 7664-93-9 H2SO4
 SOL 64-17-5 EtOH

RX(81) OF 137 COMPOSED OF RX(3), RX(16), RX(28)
 RX(81) C ==> AL



C

3
 STEPS
 →



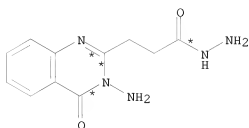
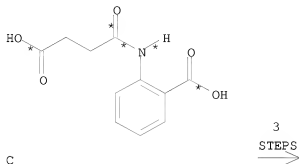
AL

RX(3) RCT C 5694-37-1
 RGT J 67-56-1 MeOH
 PRO I 54559-37-4
 CAT 7664-93-9 H2SO4
 SOL 67-56-1 MeOH

RX(16) RCT I 54559-37-4
 RGT AD 108-24-7 Ac2O
 PRO AC 54559-36-3

RX(28) RCT AC 54559-36-3
 RGT AG 302-01-2 N2H4
 PRO AL 120572-51-2
 SOL 64-17-5 EtOH

RX(83) OF 137 COMPOSED OF RX(4), RX(17), RX(29)
 RX(83) C ==> AL



AL

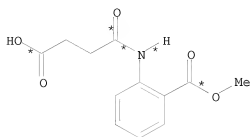
RX(4) RCT C 5694-37-1
 RGT M 64-17-5 EtOH
 PRO L 120572-36-3
 CAT 7664-93-9 H2SO4
 SOL 64-17-5 EtOH

RX(17) RCT L 120572-36-3
 RGT AD 108-24-7 Ac2O
 PRO AE 120572-46-5

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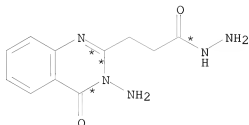
RX(29) RCT AE 120572-46-5
RGT AG 302-01-2 N2H4
PRO AL 120572-51-2
SOL 64-17-5 EtOH

RX(108) OF 137 COMPOSED OF RX(18), RX(21), RX(30)
RX(108) P ==> AL



P

3
STEPS
→



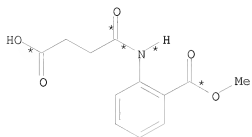
AL

RX(18) RCT P 108540-96-1
RGT AG 302-01-2 N2H4
PRO AF 84312-90-3
SOL 64-17-5 EtOH

RX(21) RCT AF 84312-90-3
RGT J 67-56-1 MeOH
PRO AI 120572-48-7
CAT 7664-93-9 H2SO4
SOL 67-56-1 MeOH

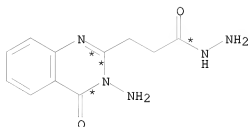
RX(30) RCT AI 120572-48-7
RGT AG 302-01-2 N2H4
PRO AL 120572-51-2
SOL 64-17-5 EtOH

RX(110) OF 137 COMPOSED OF RX(18), RX(22), RX(31)
RX(110) P ==> AL



P

3
STEPS
→



AL

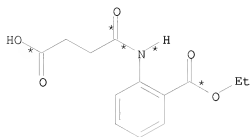
RX(18) RCT P 108540-96-1
RGT AG 302-01-2 N2H4
PRO AF 84312-90-3
SOL 64-17-5 EtOH

RX(22) RCT AF 84312-90-3
RGT M 64-17-5 EtOH
PRO AJ 120572-49-8
CAT 7664-93-9 H2SO4
SOL 64-17-5 EtOH

RX(31) RCT AJ 120572-49-8
RGT AG 302-01-2 N2H4
PRO AL 120572-51-2
SOL 64-17-5 EtOH

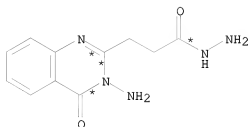
RX(112) OF 137 COMPOSED OF RX(19), RX(21), RX(30)

RX(112) R ==> AL



R

3
STEPS
→



AL

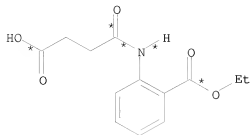
RX(19) RCT R 120572-38-5
RGT AG 302-01-2 N2H4
PRO AF 84312-90-3
SOL 64-17-5 EtOH

RX(21) RCT AF 84312-90-3
RGT J 67-56-1 MeOH
PRO AI 120572-48-7
CAT 7664-93-9 H2SO4
SOL 67-56-1 MeOH

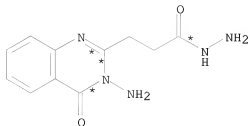
RX(30) RCT AI 120572-48-7
RGT AG 302-01-2 N2H4
PRO AL 120572-51-2
SOL 64-17-5 EtOH

RX(114) OF 137 COMPOSED OF RX(19), RX(22), RX(31)

RX(114) R ==> AL



R

3
STEPS
→

AL

RX(19) RCT R 120572-38-5
RGT AG 302-01-2 N2H4
PRO AF 84312-90-3
SOL 64-17-5 EtOH

RX(22) RCT AF 84312-90-3
RGT M 64-17-5 EtOH
PRO AJ 120572-49-8
CAT 7664-93-9 H2SO4
SOL 64-17-5 EtOH

RX(31) RCT AJ 120572-49-8
RGT AG 302-01-2 N2H4
PRO AL 120572-51-2
SOL 64-17-5 EtOH

L3 ANSWER 169 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 110:193170 CASREACT

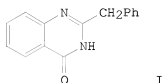
TITLE: Incorporation of molecular nitrogen into organic compounds. 2. Novel lactam synthesis by use of a combination system of carbonylation and nitrogenation
Uozumi, Yasuhiro; Kawasaki, Naofumi; Mori, Eiko; Mori, Miwako; Shibasaki, Masakatsu

CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan

SOURCE: Journal of the American Chemical Society (1989),

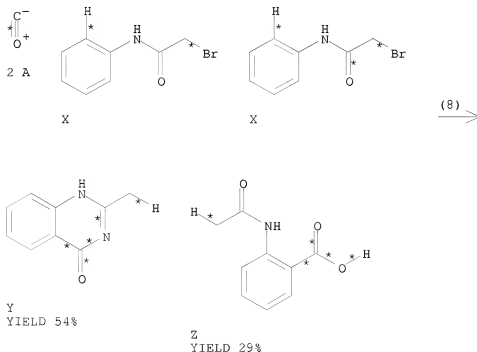
111(10), 3725-7
 CODEN: JACSAT; ISSN: 0002-7863
 Journal
 English

DOCUMENT TYPE:
 LANGUAGE:
 GI



AB An amide unit was constructed from aryl halide and a TiNCO complex under atmospheric pressure of N and CO in the presence of a Pd catalyst. With this combination of carbonylation and nitrogenation, isoindolinone and quinazolinone derivs. were synthesized from o-halophenyl alkyl ketones in one step. The reaction proceeds through the oxidative addition of enol lactone, generated by Pd-catalyzed carbonylation to o-halophenyl alkyl ketone, to TiNCO complex. Glycosminine (I) was prepared in 40% yield by this method.

RX(8) OF 9 2 A + 2 X ==> Y + Z



RX(8) RCT A 630-08-0

STAGE(1)

RGT E 7550-45-0 TiCl₄, F 7439-95-4 Mg, G 7727-37-9 N₂

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SOL 109-99-9 THF

STAGE(2)

RCT X 5326-87-4

RGT H 584-08-7 K₂CO₃

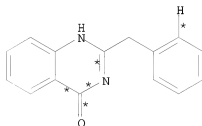
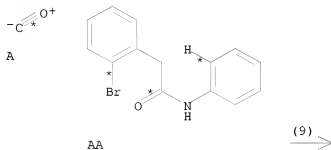
CAT 14221-01-3 Pd(PPh₃)₄

SOL 872-50-4 NMEP

PRO Y 1769-24-0, Z 89-52-1

NTE NITROGEN ACTIVATED BY TITANIUM COMPLEX

RX(9) OF 9 A + AA ==> AB



AB

YIELD 40%

RX(9) RCT A 630-08-0

STAGE(1)

RGT E 7550-45-0 TiCl₄, F 7439-95-4 Mg, G 7727-37-9 N₂

SOL 109-99-9 THF

STAGE(2)

RCT AA 120230-90-2

RGT H 584-08-7 K₂CO₃

CAT 14221-01-3 Pd(PPh₃)₄

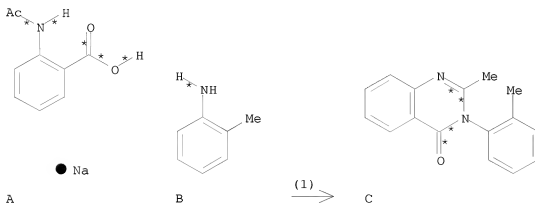
SOL 872-50-4 NMEP

PRO AB 4765-56-4

NTE NITROGEN ACTIVATED BY TITANIUM COMPLEX

L3 ANSWER 170 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 110:192758 CASREACT
 TITLE: Synthesis of some new 2-styryl-3-o-tolyl-4-quinazolone as compound of antifungal activity
 AUTHOR(S): Rawat, Malti
 CORPORATE SOURCE: Maharaja Coll., A. P. S. Univ., Rewa, India
 SOURCE: Journal of the Institution of Chemists (India) (1988), 60(2), 58
 CODEN: JOICA7; ISSN: 0020-3254
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Cyclocondensation of o-MeC₆H₄NH₂ with o-AcNHC₆H₄CO₂Na gave 2-methyl-3-o-tolyl-4-quinazolone, which reacted with PhCHO derivs. to give the title compds. These compds. were tested for fungicidal activity against *Curvularia lunata* and *Fusarium oxysporum*. The percentage of inhibition was 22.5-40.3%.

RX(1) OF 1 A + B ==> C

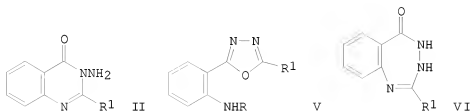


RX(1) RCT A 2870-60-2, B 95-53-4
 RGT D 7719-12-2 PC13
 PRO C 72-44-6

L3 ANSWER 171 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 110:173155 CASREACT
 TITLE: Reaction of 2-aminobenzoylhydrazines with carboxylic acids: formation of quinazolin-4(3H)-one, 1,3,4-oxadiazole and 1,3,4-benzotriazepin-5-one derivatives
 AUTHOR(S): Reddy, P. S. N.; Reddy, P. Pratap
 CORPORATE SOURCE: Dep. Chem., Osmania Univ., Hyderabad, 500 007, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1988), 27B(8), 763-5
 CODEN: IJSBDB; ISSN: 0376-4699

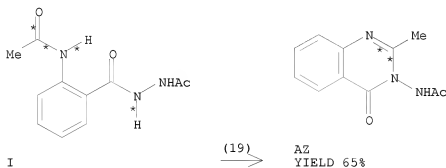
DOCUMENT TYPE:
LANGUAGE:
GI

Journal
English



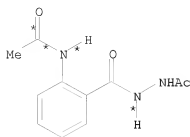
AB Reaction of 2-RNHC6H4CONHNH2 (I; R = H) with R1CO2H [R1 = H, Me, Et, Pr, Bu, Me(CH2)4] gave 2-R1CONHC6H4CONHNHCOR1, which cyclized with concentrate H2SO4 to give aminoquinazolinones II. R1CO2H (III; R1 = Ph, substituted Ph, 2-furyl, 3-pyridyl) reacted with I (R = H) to give a mixture of 2-RNHC6H4CONHNHCOR1 (IV), aryloxadiazoles V (R = H) and benzotriazepinones VI, while I (R = Me) reacted with III is given IV (R = Me) and V (R = Me).

RX(19) OF 43 ...I ==> AZ

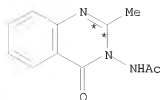


RX(19) RCT I 67571-08-8
 PRO AZ 6761-05-3
 NTE Thermal

RX(20) OF 43 I ==> AZ

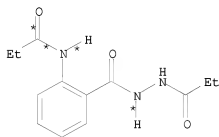


I

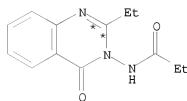
(20) \Rightarrow AZ
YIELD 81%

RX(20) RCT I 67571-08-8
 PRO AZ 6761-05-3
 CAT 104-15-4 TsOH
 SOL 1330-20-7 Xylene
 NTE Thermal

RX(21) OF 43 ...K ==> BC

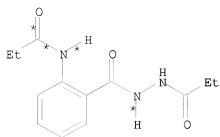


K

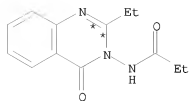
(21) \Rightarrow BC
YIELD 83%

RX(21) RCT K 67571-11-3
 PRO BC 6761-25-7
 CAT 104-15-4 TsOH
 SOL 1330-20-7 Xylene
 NTE Thermal

RX(22) OF 43 K ==> BC



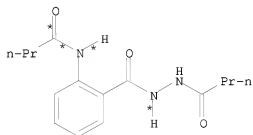
K



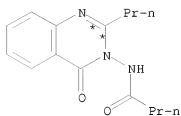
BC
YIELD 70%

RX(22) RCT K 67571-11-3
PRO BC 6761-25-7
NTE Thermal

RX(23) OF 43 ...M ==> BD



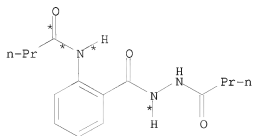
M



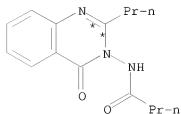
BD
YIELD 62%

RX(23) RCT M 120107-31-5
PRO BD 120107-43-9
NTE Thermal

RX(24) OF 43 M ==> BD



M

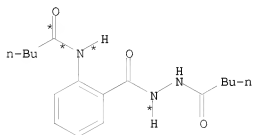


BD
YIELD 86%

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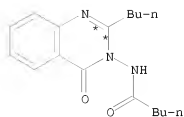
RX(24) RCT M 120107-31-5
 PRO BD 120107-43-9
 CAT 104-15-4 TsOH
 SOL 1330-20-7 Xylene
 NTE Thermal

RX(25) OF 43 ...O ==> BE



O

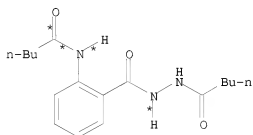
(25) \longrightarrow



BE
 YIELD 77%

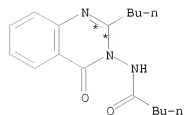
RX(25) RCT O 120107-32-6
 PRO BE 120107-44-0
 CAT 104-15-4 TsOH
 SOL 1330-20-7 Xylene
 NTE Thermal

RX(26) OF 43 O ==> BE



O

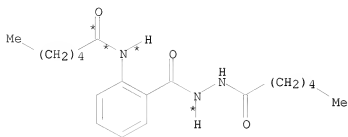
(26) \longrightarrow



BE
 YIELD 68%

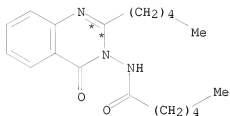
RX(26) RCT O 120107-32-6
 PRO BE 120107-44-0
 NTE Thermal

RX(27) OF 43 ...Q ==> BF



Q

(27)

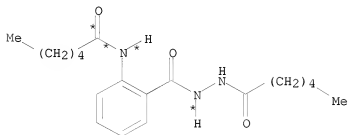


BF

YIELD 65%

RX(27) RCT Q 120107-33-7
 PRO BF 120107-45-1
 NIE Thermal

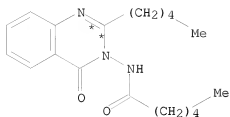
RX(28) OF 43 Q ==> BF



Q

(28)

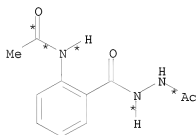
10/ 562,112



BF
YIELD 80%

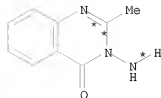
RX(28) RCT Q 120107-33-7
 PRO BF 120107-45-1
 CAT 104-15-4 TsOH
 SOL 1330-20-7 Xylene
 NTE Thermal

RX(29) OF 43 ...I ==> BG



I

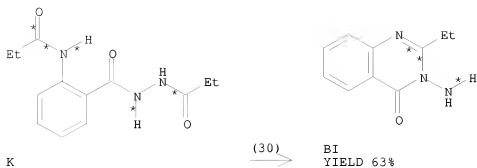
(29)
→



BG
YIELD 58%

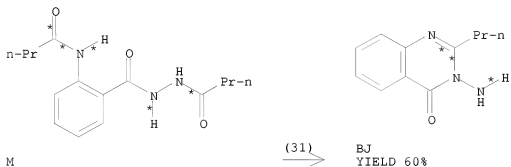
RX(29) RCT I 67571-08-8
 RGT BH 7664-93-9 H2SO4
 PRO BG 1898-06-2
 SOL 7664-93-9 H2SO4

RX(30) OF 43 ...K ==> BI



RX(30) RCT K 67571-11-3
RGT BH 7664-93-9 H2SO4
PRO BI 50547-51-8
SOL 7664-93-9 H2SO4

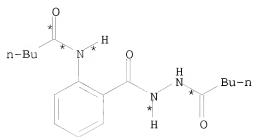
RX(31) OF 43 ...M ==> BJ



RX(31) RCT M 120107-31-5
RGT BH 7664-93-9 H2SO4
PRO BJ 84312-89-0
SOL 7664-93-9 H2SO4

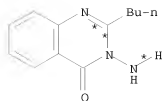
RX(32) OF 43 ...O ==> BK

10/ 562,112



O

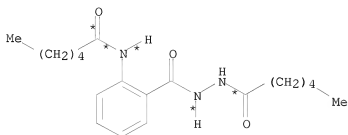
(32) \longrightarrow



BK
YIELD 64%

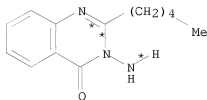
RX(32) RCT O 120107-32-6
 RGT BH 7664-93-9 H2SO4
 PRO BK 120107-46-2
 SOL 7664-93-9 H2SO4

RX(33) OF 43 ...Q ==> BL



Q

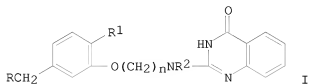
(33) \longrightarrow



BL
YIELD 55%

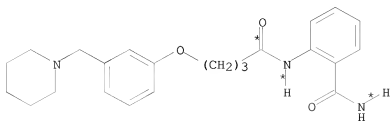
RX(33) RCT Q 120107-33-7
 RGT BH 7664-93-9 H2SO4
 PRO BL 120107-47-3
 SOL 7664-93-9 H2SO4

L3 ANSWER 172 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 110:95158 CASREACT
 TITLE: Synthesis and histamine H2-antagonist activity of 4-quinazolinone derivatives
 AUTHOR(S): Ogawa, Nobuo; Yoshida, Toshihiko; Aratani, Takayuki; Koshinaka, Eiichi; Kato, Hideo; Ito, Yasuo
 CORPORATE SOURCE: Res. Lab., Hokuriku Seiyaku Co., Ltd., Inokuchi, 911, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1988), 36(8), 2955-67
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



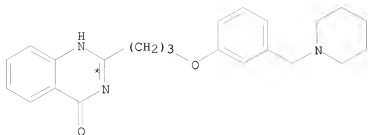
AB With the aim of developing new antiulcer agents, a series of 4-quinazolinone derivs. e.g., I (R = piperidino, pyrrolidino, morpholino, R1 = H, OMe, R2 = H, Me; n = 2, 3, 4) was synthesized and tested for histamine H2-antagonist activity and gastric antisecretory activity. Thus, 2-alkylamino-, 2-alkylthio-, and 2-alkyl-4-quinazolinones were prepared by the condensation of alkylamines with 2-chloro- or 2-methylthio-4-quinazolinones, the condensation of alkyl bromides with 2-mercapto-4-quinazolinones, and the condensation of alkylcarboxylic acids with anthranilamides, resp. Several of the 4-quinazolinone derivs. showed potent H2-antagonist activity, and one of them, I (R = piperidino, R1 = R2 = H, n = 3), showed the most potent antisecretory activity. The structure-activity relationships are discussed.

RX(49) OF 95 ...Y ==> DJ



Y

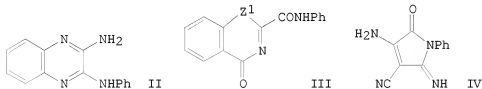
(49) →



DJ

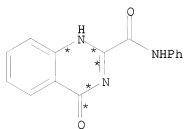
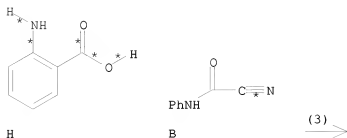
RX(49) RCT Y 119023-27-7
 RGT V 1310-73-2 NaOH
 PRO DJ 105189-23-9
 SOL 67-56-1 MeOH, 7732-18-5 Water

L3 ANSWER 173 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 110:38956 CASREACT
 TITLE: Nitriles in heterocyclic synthesis:
 1-cyanoformanilide as precursor for a variety of
 heterocyclic ring systems
 AUTHOR(S): Sherif, Sherif Mourad; Mohareb, Rafaat Milad;
 Elgemeie, Galal Eldin H.; Singh, Rajendra Prasad
 CORPORATE SOURCE: Fac. Sci., Cairo Univ., Giza, Egypt
 SOURCE: Heterocycles (1988), 27(7), 1579-83
 CODEN: HTCYAM; ISSN: 0385-5414
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB PhNHCOCN (I) was converted to quinoxaline derivative II and other heterocycles III (Z1 = O, NH). I was treated with o-phenylenediamine in DMF containing piperidine to give II. III (Z1 = O) was prepared from I, salicylic acid, and Et3N in EtOH. Pyrrolinone IV was obtained from I and CH2(CN)2.

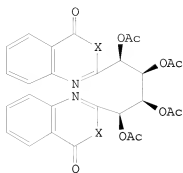
RX(3) OF 10 H + B ==> I



I

RX(3) RCT H 118-92-3, B 6784-22-1
 PRO I 118372-87-5
 CAT 121-44-8 Et3N
 SOL 64-17-5 EtOH

L3 ANSWER 174 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 109:231445 CASREACT
 TITLE: Heterocycles from carbohydrate precursors. Part 46.
 A novel approach for the synthesis of C-nucleoside
 analogs by constructing benzoxazine rings linked to a
 carbohydrate moiety
 AUTHOR(S): El Ashry, El Sayed H.; Rashed, Nagwa; Mousaad, Ahmed
 CORPORATE SOURCE: Fac. Sci., Alexandria Univ., Alexandria, Egypt
 SOURCE: Journal of Carbohydrate Chemistry (1987), 6(4),
 599-607
 CODEN: JCACDM; ISSN: 0732-8303
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

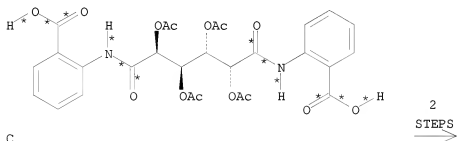


I

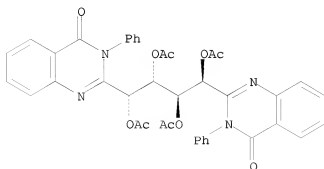
AB Dehydrative cyclization of the condensation product of 2,3,4,5-tetra-O-acetyl-galactaryl chloride with anthranilic acid gave 1,2,3,4-tetra-O-acetyl-1,4-bis(4H-benzoxazin-4-one-2-yl)-galacto-tetritol (I, X = O). Its reaction with PhNH₂ in the presence of PCl₃ afforded 1,4-bis(3-phenylquinazolin-4-one-2-yl)-1,2,3,4-tetra-O-acetyl-galacto-tetritol (I, X = NPh).

RX(9) OF 11 COMPOSED OF RX(2), RX(6)

RX(9) C ==> K



C



K

YIELD 77%

RX(2) RCT C 82185-59-9

RGT G 108-24-7 Ac2O
PRO F 82185-60-2

RX(6) RCT F 82185-60-2
RGT L 7719-12-2 PC13
PRO K 117641-26-6
SOL 108-88-3 PhMe

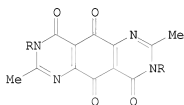
L3 ANSWER 175 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 109:128947 CASREACT
TITLE: Synthesis and electrochemistry of
pyrimidoquinazoline-5,10-diones. Design of
hydrolytically stable high potential quinones and new
reductive alkylation systems

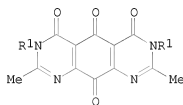
AUTHOR(S): Skibo, Edward B.; Gilchrist, James H.
CORPORATE SOURCE: Dep. Chem., Arizona State Univ., Tempe, AZ,
85287-1604, USA

SOURCE: Journal of Organic Chemistry (1988), 53(18), 4209-18
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

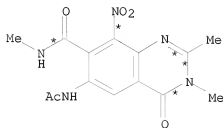
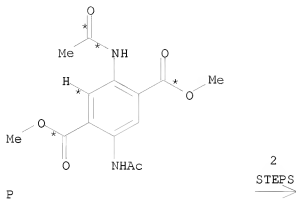


II

AB The synthesis of pyrimido[4,5-g]quinazoline-5,10-diones I (R = H, Me) and pyrimido[5,4-g]quinazoline-5,10-diones II (R1 = H, Me) was carried out in conjunction with the design of both hydrolytically stable high potential quinones and new purine-like reductive alkylating agents. I and II consist of a benzoquinone ring bearing two fused pyrimidinone rings. The fused pyrimidinone rings serve to protect I and II from hydrolysis as well as to raise quinone redox potentials by stabilizing the hydroquinones with internal H bonds (65 mV increase per H bond). Synthesis of I and II involved pyrimidinone ring annulation to a 2,5-diamino-3-nitroterephthalic acid derivative and to a 2,4-diamino-1,5-dicarboxy-3-nitrobenzene derivative, resp. The synthetic studies provided insights into the electronic effects of nitro and amino groups on the annulation process.

RX(36) OF 141 COMPOSED OF RX(7), RX(8)
RX(36) P ==> U

10/ 562,112



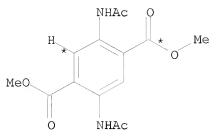
U
YIELD 51%

RX(7) RCT P 115705-52-7
RGT T 50-00-0 HCHO, J 7697-37-2 HNO3
PRO S 115705-53-8
SOL 7697-37-2 HNO3

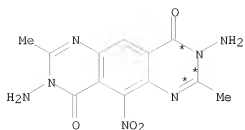
RX(8) RCT S 115705-53-8
RGT V 74-89-5 MeNH2
PRO U 115705-55-0
SOL 68-12-2 DMF, 67-56-1 MeOH

RX(37) OF 141 COMPOSED OF RX(7), RX(10)
RX(37) P + Y ==> Z

10/ 562,112

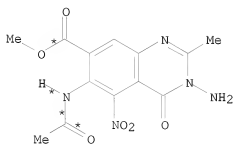


P



Y

2
STEPS
→

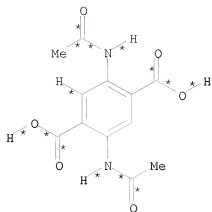


Z
YIELD 69%

RX(7) RCT P 115705-52-7
RGT T 50-00-0 HCHO, J 7697-37-2 HNO3
PRO S 115705-53-8
SOL 7697-37-2 HNO3

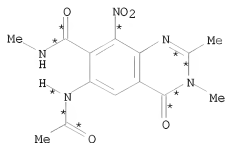
RX(10) RCT S 115705-53-8, Y 115705-56-1
RGT AA 302-01-2 N2H4
PRO Z 115705-54-9
SOL 67-56-1 MeOH

RX(67) OF 141 COMPOSED OF RX(5), RX(6), RX(7), RX(8)
RX(67) M ==> U



M

4
STEPS
→



U
YIELD 51%

RX(5) RCT M 115705-51-6
 RGT L 108-24-7 Ac2O
 PRO N 22438-03-5
 SOL 64-19-7 AcOH, 108-24-7 Ac2O

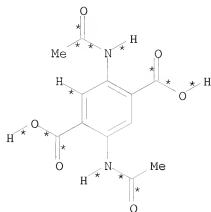
RX(6) RCT N 22438-03-5
 RGT Q 124-41-4 NaOMe
 PRO P 115705-52-7
 SOL 67-56-1 MeOH

RX(7) RCT P 115705-52-7
 RGT T 50-00-0 HCHO, J 7697-37-2 HNO3
 PRO S 115705-53-8
 SOL 7697-37-2 HNO3

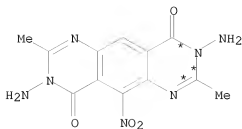
RX(8) RCT S 115705-53-8
 RGT V 74-89-5 MeNH2
 PRO U 115705-55-0
 SOL 68-12-2 DMF, 67-56-1 MeOH

RX(68) OF 141 COMPOSED OF RX(5), RX(6), RX(7), RX(10)

RX(68) M + Y ==> Z

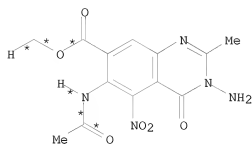


M



Y

4
STEPS
→



Z

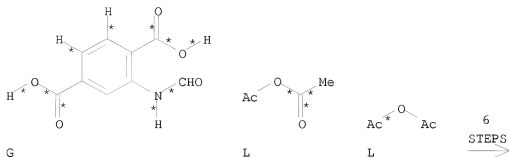
YIELD 69%

- RX(5) RCT M 115705-51-6
RGT L 108-24-7 Ac₂O
PRO N 22438-03-5
SOL 64-19-7 AcOH, 108-24-7 Ac₂O
- RX(6) RCT N 22438-03-5
RGT Q 124-41-4 NaOMe
PRO P 115705-52-7
SOL 67-56-1 MeOH
- RX(7) RCT P 115705-52-7
RGT T 50-00-0 HCHO, J 7697-37-2 HNO₃
PRO S 115705-53-8
SOL 7697-37-2 HNO₃
- RX(10) RCT S 115705-53-8, Y 115705-56-1
RGT AA 302-01-2 N₂H₄
PRO Z 115705-54-9
SOL 67-56-1 MeOH

RX(105) OF 141 COMPOSED OF RX(3), RX(4), RX(5), RX(6), RX(7), RX(8)

10/ 562,112

RX(105) G + 2 L ==> U



U
YIELD 51%

RX(3) RCT G 115705-49-2
RGT J 7697-37-2 HNO3, K 7664-93-9 H2SO4
PRO I 115705-50-5
SOL 7697-37-2 HNO3, 7664-93-9 H2SO4

RX(4) RCT I 115705-50-5, L 108-24-7
RGT C 1333-74-0 H2, D 1310-58-3 KOH
PRO M 115705-51-6
CAT 7440-05-3 Pd
SOL 7732-18-5 Water

RX(5) RCT M 115705-51-6
RGT L 108-24-7 Ac2O
PRO N 22438-03-5
SOL 64-19-7 AcOH, 108-24-7 Ac2O

RX(6) RCT N 22438-03-5
RGT Q 124-41-4 NaOMe
PRO P 115705-52-7
SOL 67-56-1 MeOH

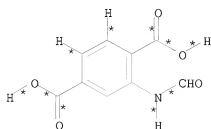
RX(7) RCT P 115705-52-7
RGT T 50-00-0 HCHO, J 7697-37-2 HNO3
PRO S 115705-53-8
SOL 7697-37-2 HNO3

RX(8) RCT S 115705-53-8

10/ 562,112

RGT V 74-89-5 MeNH2
 PRO U 115705-55-0
 SOL 68-12-2 DMF, 67-56-1 MeOH

RX(106) OF 141 COMPOSED OF RX(3), RX(4), RX(5), RX(6), RX(7), RX(10)
 RX(106) G + 2 L + Y ==> Z



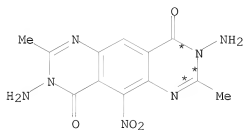
G



L

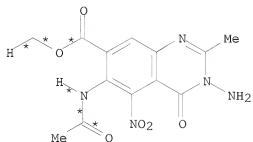


L



Y

6
 STEPS
 >



Z

YIELD 69%

RX(3) RCT G 115705-49-2
 RGT J 7697-37-2 HNO3, K 7664-93-9 H2SO4
 PRO I 115705-50-5
 SOL 7697-37-2 HNO3, 7664-93-9 H2SO4

RX(4) RCT I 115705-50-5, L 108-24-7
 RGT C 1333-74-0 H2, D 1310-58-3 KOH
 PRO M 115705-51-6
 CAT 7440-05-3 Pd
 SOL 7732-18-5 Water

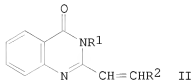
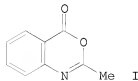
RX(5) RCT M 115705-51-6
 RGT L 108-24-7 Ac2O
 PRO N 22438-03-5
 SOL 64-19-7 AcOH, 108-24-7 Ac2O

RX(6) RCT N 22438-03-5
 RGT Q 124-41-4 NaOMe
 PRO P 115705-52-7
 SOL 67-56-1 MeOH

RX(7) RCT P 115705-52-7
 RGT T 50-00-0 HCHO, J 7697-37-2 HNO3
 PRO S 115705-53-8
 SOL 7697-37-2 HNO3

RX(10) RCT S 115705-53-8, Y 115705-56-1
 RGT AA 302-01-2 N2H4
 PRO Z 115705-54-9
 SOL 67-56-1 MeOH

L3 ANSWER 176 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 109:92923 CASREACT
 TITLE: One-pot conversion of 2-methyl-3,1-benzoxazin-4-one
 into 3-substituted-2-styrylquinazolin-4-ones
 AUTHOR(S): Jain, Archana; Mukerjee, Arya K.
 CORPORATE SOURCE: Fac. Sci., Banaras Hindu Univ., Varanasi, 221 005,
 India
 SOURCE: Journal of the Indian Chemical Society (1987), 64(10),
 645-6
 CODEN: JICSAH; ISSN: 0019-4522
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

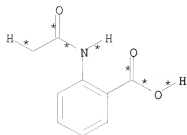


AB Benzoxazinone I was treated with R1NH2 (R1 = Ph, ClC6H4, anisyl, HO2CC6H4) and R2CHO [R2 = Ph, HOC6H4, HO(MeO)C6H3] to give styrylquinazolinones II. The treatment of 2-AcNHC6H4CO2H with tosyl chloride and Et3N gave I.

RX(8) OF 13 COMPOSED OF RX(1), RX(2)

10/ 562,112

RX(8) A + F + G ==> H



A

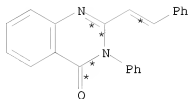


F



G

2
STEPS
→



H

RX(1) RCT A 89-52-1
 RGT C 98-59-9 TsCl, D 121-44-8 Et3N
 PRO B 525-76-8
 SOL 71-43-2 Benzene

RX(2) RCT B 525-76-8, F 62-53-3

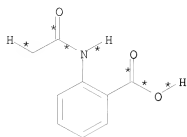
STAGE(1)
SOL 64-19-7 AcOH

STAGE(2)
RCT G 100-52-7
CAT 127-09-3 AcONa

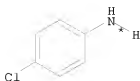
PRO H 77143-60-3

RX(9) OF 13 COMPOSED OF RX(1), RX(3)

RX(9) A + K + G ==> L



A

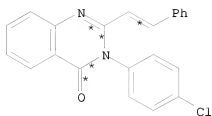


K



G

2
STEPS
→



L

RX(1) RCT A 89-52-1
RGT C 98-59-9 TsCl, D 121-44-8 Et3N
PRO B 525-76-8
SOL 71-43-2 Benzene

RX(3) RCT B 525-76-8, K 106-47-8

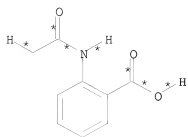
STAGE(1)
SOL 64-19-7 AcOH

STAGE(2)
RCT G 100-52-7
CAT 127-09-3 AcONa

PRO L 115781-69-6

RX(10) OF 13 COMPOSED OF RX(1), RX(4)

RX(10) A + M + G ==> N



A

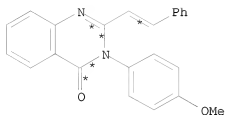


M



G

2
STEPS
→



N

RX(1) RCT A 89-52-1
RGT C 98-59-9 TsCl, D 121-44-8 Et3N
PRO B 525-76-8
SOL 71-43-2 Benzene

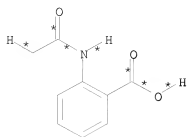
RX(4) RCT B 525-76-8, M 104-94-9

STAGE(1)
SOL 64-19-7 AcOH

STAGE(2)
RCT G 100-52-7
CAT 127-09-3 AcONa

PRO N 115781-70-9

RX(11) OF 13 COMPOSED OF RX(1), RX(5)
RX(11) A + O + G ==> P



A

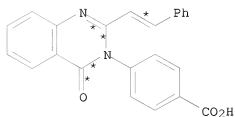


O



G

2
STEPS
→



P

RX(1) RCT A 89-52-1
RGT C 98-59-9 TsCl, D 121-44-8 Et3N
PRO B 525-76-8
SOL 71-43-2 Benzene

RX(5) RCT B 525-76-8, O 150-13-0

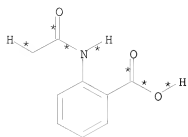
STAGE(1)
SOL 64-19-7 AcOH

STAGE(2)
RCT G 100-52-7
CAT 127-09-3 AcONa

PRO P 37856-33-0

RX(12) OF 13 COMPOSED OF RX(1), RX(6)

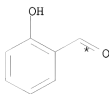
RX(12) A + F + Q ==> R



A

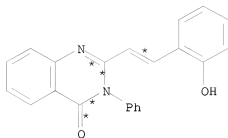


F



Q

2
STEPS
→



R

RX(1) RCT A 89-52-1
RGT C 98-59-9 TsCl, D 121-44-8 Et3N
PRO B 525-76-8
SOL 71-43-2 Benzene

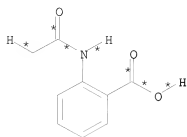
RX(6) RCT B 525-76-8, F 62-53-3

STAGE(1)
SOL 64-19-7 AcOH

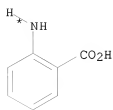
STAGE(2)
RCT Q 90-02-8
CAT 127-09-3 AcONa

PRO R 77815-33-9

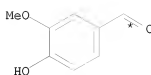
RX(13) OF 13 COMPOSED OF RX(1), RX(7)
RX(13) A + S + T ==> U



A

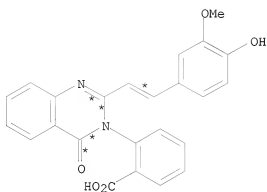


S



T

2
STEPS
→



U

RX(1) RCT A 89-52-1
RGT C 98-59-9 TsCl, D 121-44-8 Et3N
PRO B 525-76-8
SOL 71-43-2 Benzene

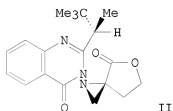
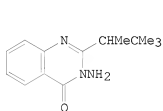
RX(7) RCT B 525-76-8, S 118-92-3

STAGE(1)
SOL 64-19-7 AcOH

STAGE(2)
RCT T 121-33-5
CAT 127-09-3 AcONa

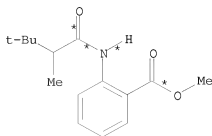
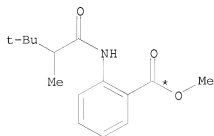
PRO U 72743-31-8

L3 ANSWER 177 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 109:92918 CASREACT
 TITLE: Asymmetric induction in addition of N-nitrenes to alkenes. Oxidation of 3-amino-2-(1,2,2-trimethylpropyl)quinazolin-4(3H)-one in the presence of α -methylene- γ -butyrolactone: conformation analysis of the aziridines formed and comparison with alkanoylated cyclopropylamines
 AUTHOR(S): Atkinson, Robert S.; Tughan, Gary
 CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (12), 2797-802
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

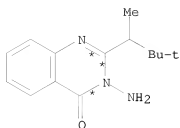


AB Oxidation of the title N-aminoquinazolinone (I) in the presence of α -methylene- γ -butyrolactone yields the spiroaziridines II with virtually no asym. induction. The same oxidation carried out in the presence of 3.4 mol. equivalent of CF₃CO₂H yielded only a single stereoisomer. The mol. structure reveals an unexpected orientation around the N-N bond by comparison with other hydrazines. The NMR spectra of the isomers of II show that both aziridines exist in solution as single invertomers at nitrogen: one isomer shows the presence of both rotamers around the N-N bond, but only one rotamer is evident for the other.

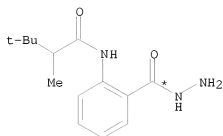
RX(5) OF 24 2 0 ==> A + P...



(5) →



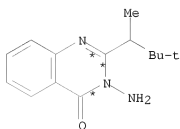
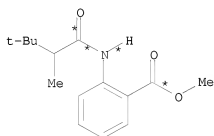
A
YIELD 24%



P
YIELD 55%

RX(5) RCT O 115875-69-9
RGT Q 302-01-2 N2H4
PRO A 116065-10-2, P 115855-35-1
SOL 64-17-5 EtOH

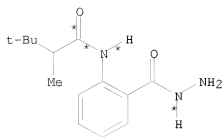
RX(7) OF 24 0 ==> A...


$$O \xrightarrow{(7)} A$$

YIELD 74%

RX (7)	RCT	O 115875-69-9
	RGT	Q 302-01-2 N2H4
	PRO	A 116065-10-2
	SOL	64-17-5 EtOH

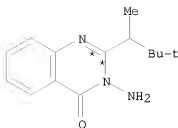
RX(9) OF 24 . . . P ==> A . . .



P

(9) \Rightarrow

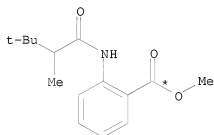
A



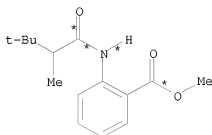
RX(9) RCT P 115855-35-1
 PRO A 116065-10-2
 SOL 64-17-5 EtOH

RX(11) OF 24 COMPOSED OF RX(5), RX(1)

RX(11) 2 O + B \Rightarrow C



O



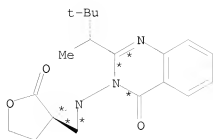
O



B

2
 STEPS
 \Rightarrow

10/ 562,112

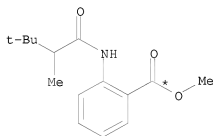


C
YIELD 72%

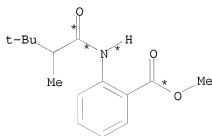
RX(5) RCT O 115875-69-9
 RGT Q 302-01-2 N2H4
 PRO A 116065-10-2, P 115855-35-1
 SOL 64-17-5 EtOH

RX(1) RCT A 116065-10-2, B 547-65-9
 RGT D 546-67-8 Pb(OAc)4, E 76-05-1 F3CCO2H
 PRO C 105983-10-6
 SOL 75-09-2 CH2Cl2

RX(12) OF 24 COMPOSED OF RX(5), RX(2)
RX(12) 3 O + 2 B ==> C + G



O

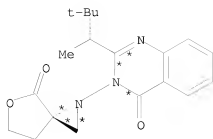


2 O

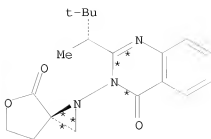


2 B

2
STEPS
=>



C



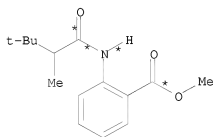
G

RX(5) RCT O 115875-69-9
 RGT Q 302-01-2 N2H4
 PRO A 116065-10-2, P 115855-35-1
 SOL 64-17-5 EtOH

RX(2) RCT A 116065-10-2, B 547-65-9
 RGT D 546-67-8 Pb(OAc)4
 PRO C 105983-10-6, G 105983-09-3
 SOL 75-09-2 CH2Cl2

RX(13) OF 24 COMPOSED OF RX(7), RX(1)

RX(13) O + B ==> C

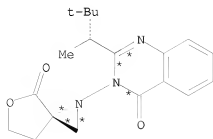


O



B

2
 STEPS
 →



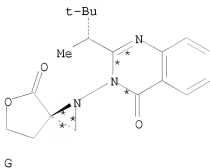
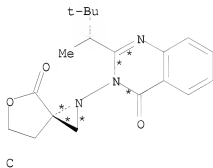
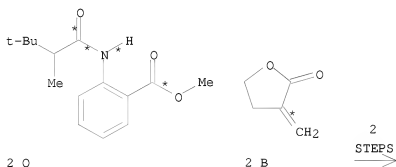
C

YIELD 72%

RX(7) RCT O 115875-69-9
 RGT Q 302-01-2 N2H4
 PRO A 116065-10-2
 SOL 64-17-5 EtOH

RX(1) RCT A 116065-10-2, B 547-65-9
 RGT D 546-67-8 Pb(OAc)4, E 76-05-1 F3CCO2H
 PRO C 105983-10-6
 SOL 75-09-2 CH2Cl2

RX(14) OF 24 COMPOSED OF RX(7), RX(2)
 RX(14) 2 O + 2 B ==> C + G

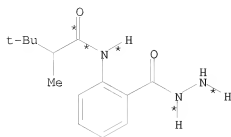


RX(7) RCT O 115875-69-9
 RGT Q 302-01-2 N2H4
 PRO A 116065-10-2
 SOL 64-17-5 EtOH

RX(2) RCT A 116065-10-2, B 547-65-9
 RGT D 546-67-8 Pb(OAc)4
 PRO C 105983-10-6, G 105983-09-3
 SOL 75-09-2 CH2Cl2

RX(15) OF 24 COMPOSED OF RX(9), RX(1)
 RX(15) P + B ==> C

10/ 562,112

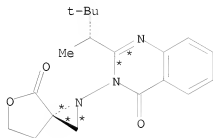


P



B

2
STEPS
→



C

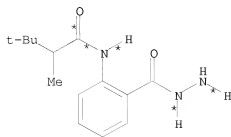
YIELD 72%

RX(9) RCT P 115855-35-1
PRO A 116065-10-2
SOL 64-17-5 EtOH

RX(1) RCT A 116065-10-2, B 547-65-9
RGT D 546-67-8 Pb(OAc)4, E 76-05-1 F3CCO2H
PRO C 105983-10-6
SOL 75-09-2 CH2Cl2

RX(16) OF 24 COMPOSED OF RX(9), RX(2)

RX(16) 2 P + 2 B ==> C + G

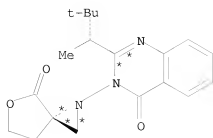


2 P

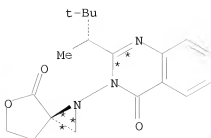


2 B

2
STEPS
→



C

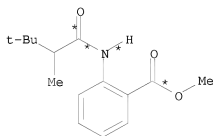


G

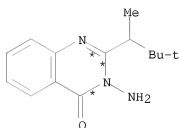
RX(9) RCT P 115855-35-1
 PRO A 116065-10-2
 SOL 64-17-5 EtOH

RX(2) RCT A 116065-10-2, B 547-65-9
 RGT D 546-67-8 Pb(OAc)₄
 PRO C 105983-10-6, G 105983-09-3
 SOL 75-09-2 CH₂Cl₂

RX(17) OF 24 COMPOSED OF RX(5), RX(9)
 RX(17) 2 O ==> A



2 O



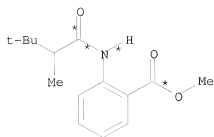
A

RX(5) RCT O 115875-69-9
 RGT Q 302-01-2 N₂H₄
 PRO A 116065-10-2, P 115855-35-1
 SOL 64-17-5 EtOH

RX(9) RCT P 115855-35-1
 PRO A 116065-10-2
 SOL 64-17-5 EtOH

RX(21) OF 24 COMPOSED OF RX(5), RX(9), RX(1)
 RX(21) 2 O + B ==> C

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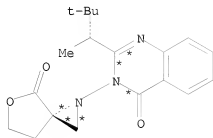


2 O



B

3
STEPS
→



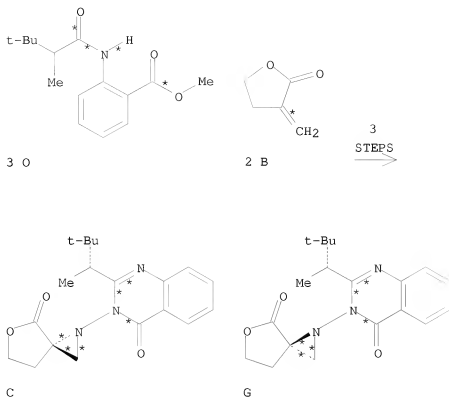
C

YIELD 72%

RX(5)	RCT	O 115875-69-9
	RGT	Q 302-01-2 N2H4
	PRO	A 116065-10-2, P 115855-35-1
	SOL	64-17-5 EtOH
RX(9)	RCT	P 115855-35-1
	PRO	A 116065-10-2
	SOL	64-17-5 EtOH
RX(1)	RCT	A 116065-10-2, B 547-65-9
	RGT	D 546-67-8 Pb(OAc)4, E 76-05-1 F3CCO2H
	PRO	C 105983-10-6
	SOL	75-09-2 CH2Cl2

RX(22) OF 24 COMPOSED OF RX(5), RX(9), RX(2)

RX(22) 3 O + 2 B ==> C + G

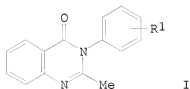


RX(5)	RCT	O 115875-69-9
	RGT	Q 302-01-2 N2H4
	PRO	A 116065-10-2, P 115855-35-1
	SOL	64-17-5 EtOH
RX(9)	RCT	P 115855-35-1
	PRO	A 116065-10-2
	SOL	64-17-5 EtOH
RX(2)	RCT	A 116065-10-2, B 547-65-9
	RGT	D 546-67-8 Pb(OAc)4
	PRO	C 105983-10-6, G 105983-09-3
	SOL	75-09-2 CH2Cl2

L3 ANSWER 178 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 108:186690 CASREACT
 TITLE: Phosphorus pentoxide in organic synthesis. XXX. New
 synthesis of 4(3H)-quinazolinones
 AUTHOR(S): Hilmy, Khalid Mohamed Hassan; Mogensen, Joergen;
 Pedersen, Erik B.
 CORPORATE SOURCE: Dep. Chem., Odense Univ., Odense, DK-5230, Den.
 SOURCE: Acta Chemica Scandinavica, Series B: Organic
 Chemistry and Biochemistry (1987), B41(6), 467-8
 CODEN: ACBOCV; ISSN: 0302-4369

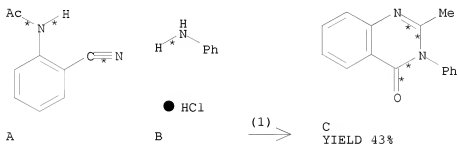
DOCUMENT TYPE:
LANGUAGE:
GI

Journal
English



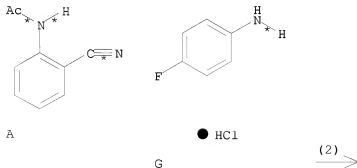
AB Aniline salts $R_1C_6H_4NH_2.HCl$ ($R_1 = H, F, Cl, Me$) were heated with P_2O_5 , water, and N,N -dimethylcyclohexylamine hydrochloride to give quinazolinones I.

RX(1) OF 10 A + B ==> C

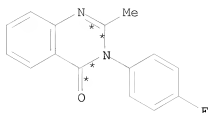


RX(1) RCT A 25116-00-1, B 142-04-1
RGT D 1314-56-3 P_2O_5 , E 2498-24-0 $Me_2NC_6H_{11}.HCl$, F 7732-18-5 Water
PRO C 2385-23-1

RX(2) OF 10 A + G ==> H



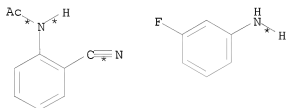
10/ 562,112



H
YIELD 37%

RX(2) RCT A 25116-00-1, G 2146-07-8
RGT D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water
PRO H 1897-80-9

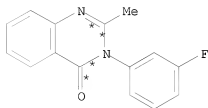
RX(3) OF 10 A + I ==> J



A ● HCl

I

(3) →

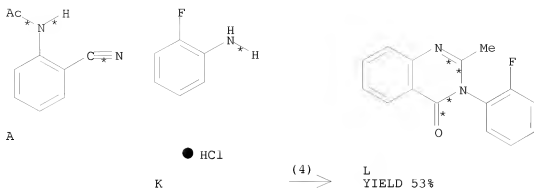


J
YIELD 46%

RX(3) RCT A 25116-00-1, I 1993-09-5
RGT D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water
PRO J 1789-04-4

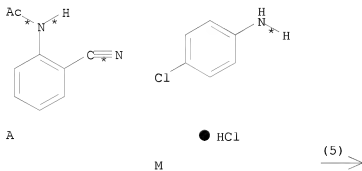
RX(4) OF 10 A + K ==> L

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RX(4) RCT A 25116-00-1, K 51085-49-5
 RGT D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water
 PRO L 1897-87-6

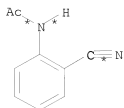
RX(5) OF 10 A + M \Rightarrow N



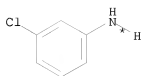
N
 YIELD 50%

RX(5) RCT A 25116-00-1, M 20265-96-7
 RGT D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water
 PRO N 1788-93-8

RX(6) OF 10 A + O \Rightarrow P

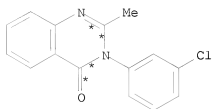


A



Q

● HCl

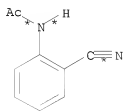


P

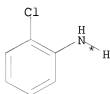
YIELD 38%

RX(6) RCT A 25116-00-1, O 141-85-5
 RGT D 1314-56-3 P205, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water
 PRO P 340-94-3

RX(7) OF 10 A + Q ==> R

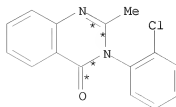


A



Q

● HCl



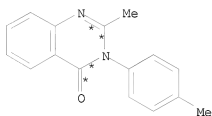
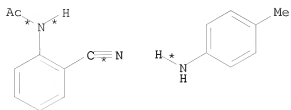
R

YIELD 31%

RX(7) RCT A 25116-00-1, Q 137-04-2
 RGT D 1314-56-3 P205, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water
 PRO R 340-57-8

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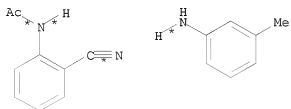
RX(8) OF 10 A + S ==> T

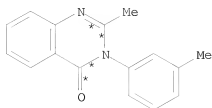


T
YIELD 33%

RX(8) RCT A 25116-00-1, S 540-23-8
 RGT D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water
 PRO T 22316-59-2

RX(9) OF 10 A + U ==> V

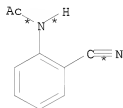




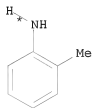
V
YIELD 40%

RX(9) RCT A 25116-00-1, U 638-03-9
RGT D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water
PRO V 22288-99-9

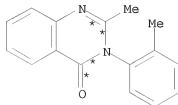
RX(10) OF 10 A + W ==> X



A



● HCl
W



X
YIELD 53%

RX(10) RCT A 25116-00-1, W 636-21-5
RGT D 1314-56-3 P2O5, E 2498-24-0 Me2NC6H11.HCl, F 7732-18-5 Water
PRO X 72-44-6

L3 ANSWER 179 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 108:56047 CASREACT

TITLE: Some reactions of
N-[(3,4-dimethylbenzoyl)acryloyl]anthranilic acid and
its derivatives

AUTHOR(S): Soliman, E. A.; Hataba, A. M.; Attia, I. A.;
El-Shahed, F. A.; Mousa, H. A.

CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt

SOURCE: Journal of the Chemical Society of Pakistan (1987),
9(1), 19-34

CODEN: JCSPDF; ISSN: 0253-5106

DOCUMENT TYPE: Journal

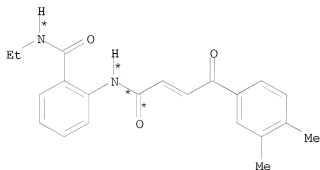
10/ 562,112

LANGUAGE: English
GI

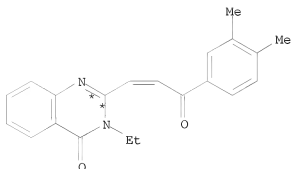
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Cyclization of anthranilic acid derivative I with $\text{RNHC}(\text{Z})\text{NH}_2$ ($\text{R} = \text{H}$, $\text{Z} = \text{O}$, S ; $\text{R} = \text{PhCH}_2$, $\text{Z} = \text{S}$) and with Ac_2O gave pyrimidines II ($\text{R} = \text{H}$, PhCH_2 ; $\text{Z} = \text{O}$, S) and benzoxazinone III, resp. Cyclocondensation of III with N_2H_4 gave aminoquinazolinone IV ($\text{R}_1 = \text{H}$). Condensation of III with N_2H_4 in the presence of $\text{R}_2\text{CO}_2\text{H}$ ($\text{R}_2 = \text{H}$, Me , Et , Pr) gave IV ($\text{R}_1 = \text{COR}_2$). Some reactions of IV ($\text{R}_1 = \text{H}$) were also investigated.

RX(12) OF 122 ...V ==> AC



V

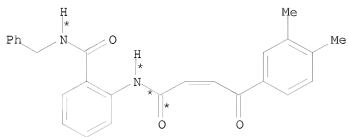


AC
YIELD 50%

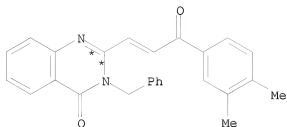
RX(12) RCT V 112371-81-0
RGT R 108-24-7 Ac2O
PRO AC 112371-77-4
SOL 108-24-7 Ac2O

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RX(14) OF 122 ...Z ==> AD



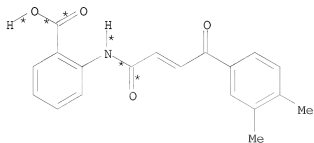
Z



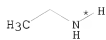
AD
YIELD 55%

RX(14) RCT Z 112371-79-6
RGT R 108-24-7 Ac2O
PRO AD 112371-76-3
SOL 108-24-7 Ac2O

RX(49) OF 122 COMPOSED OF RX(6), RX(13)
RX(49) C + U ==> AC



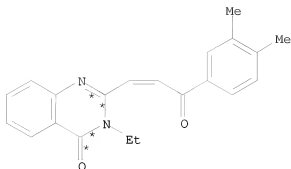
C



U



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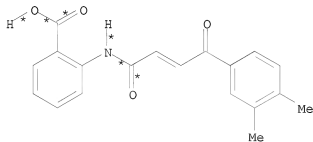


AC
YIELD 50%

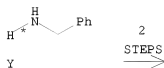
RX(6) RCT C 112371-88-7
 RGT R 108-24-7 Ac2O
 PRO Q 112371-83-2
 SOL 108-24-7 Ac2O

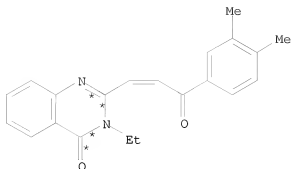
RX(13) RCT Q 112371-83-2, U 75-04-7
 RGT AA 124-40-3 Me2NH
 PRO AC 112371-77-4

RX(50) OF 122 COMPOSED OF RX(6), RX(15)
RX(50) C + Y ==> AD



C





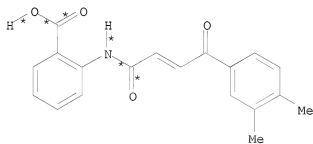
AC
YIELD 50%

RX(6) RCT C 112371-88-7
RGT R 108-24-7 Ac2O
PRO Q 112371-83-2
SOL 108-24-7 Ac2O

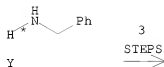
RX(8) RCT Q 112371-83-2, U 75-04-7
PRO V 112371-81-0
SOL 64-17-5 EtOH

RX(12) RCT V 112371-81-0
RGT R 108-24-7 Ac2O
PRO AC 112371-77-4
SOL 108-24-7 Ac2O

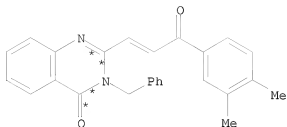
RX(94) OF 122 COMPOSED OF RX(6), RX(10), RX(14)
RX(94) C + Y ==> AD



C



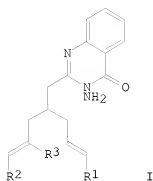
3
STEPS
→



AD
YIELD 55%

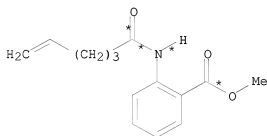
RX(6)	RCT	C 112371-88-7
	RGT	R 108-24-7 Ac2O
	PRO	Q 112371-83-2
	SOL	108-24-7 Ac2O
RX(10)	RCT	Q 112371-83-2, Y 100-46-9
	PRO	Z 112371-79-6
	SOL	64-17-5 EtOH
RX(14)	RCT	Z 112371-79-6
	RGT	R 108-24-7 Ac2O
	PRO	AD 112371-76-3
	SOL	108-24-7 Ac2O

L3 ANSWER 180 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 108:56028 CASREACT
 TITLE: Intramolecular reactions of N-nitrenes. Description of the transition state geometry for addition to alkenes
 AUTHOR(S): Atkinson, Roberts S.; Grimshire, Michael J.
 CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (5), 1127-37
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

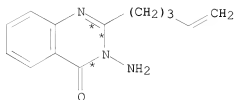


AB Oxidation of the N-aminoquinazolones I ($R_1 = R_3 = H$, $R_2 = Ph$; $R_1 = R_3 = Me$, $R_2 = H$) by $Pb(OAc)_4$ generates the corresponding N-nitrenes which add intramolecularly to both double bonds. Although nitrene addition is stereospecifically cis, both faces of each double bond are attacked and consequently stereoisomers are formed. From the different selectivity of the N-nitrenes for the two double bonds in I and from a consideration of the stereoisomer ratios, a transition-state is proposed for the concerted addition of the N-nitrene to the double bonds in (I).

RX(26) OF 204 ...AT ==> AV...



AT



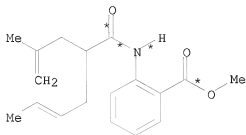
AV
YIELD 80%

RX(26) RCT AT 112391-61-4

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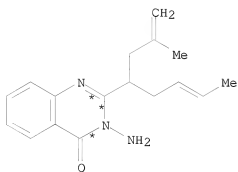
RGT AW 302-01-2 N2H4
PRO AV 112391-72-7
SOL 64-17-5 EtOH

RX(27) OF 204 ...AX ==> AY...



AX

(27)

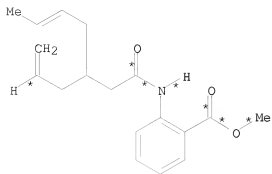


AY
YIELD 90%

RX(27) RCT AX 112391-62-5
RGT AW 302-01-2 N2H4
PRO AY 112391-73-8
SOL 64-17-5 EtOH

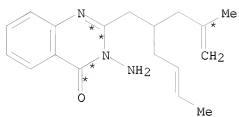
RX(28) OF 204 ...AZ ==> BA...

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AZ

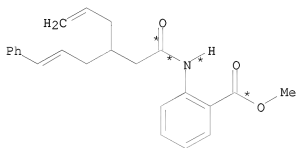
(28) \Rightarrow



BA

RX(28) RCT AZ 112391-63-6
 RGT AW 302-01-2 N2H4
 PRO BA 101126-05-0
 SOL 64-17-5 EtOH

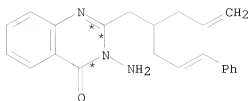
RX(29) OF 204 ...BB \Rightarrow BC...



BB

(29) \Rightarrow

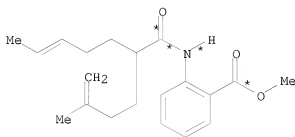
10/ 562,112



BC
YIELD 41%

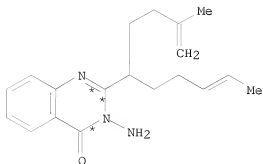
RX(29) RCT BB 112391-64-7
 RGT AW 302-01-2 N2H4
 PRO BC 101126-02-7
 SOL 64-17-5 EtOH

RX(30) OF 204 ...BD ==> BE...



BD

(30)
→

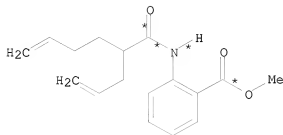


BE
YIELD 47%

RX(30) RCT BD 112391-65-8
 RGT AW 302-01-2 N2H4
 PRO BE 112391-74-9
 SOL 64-17-5 EtOH

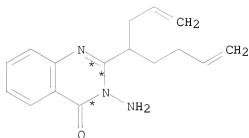
10/ 562,112

RX(31) OF 204 ...BF ==> BG...



BF

(31)
→

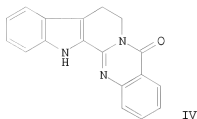
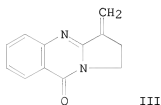
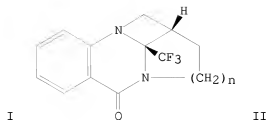
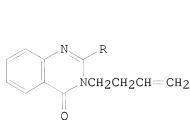


BG

YIELD 56%

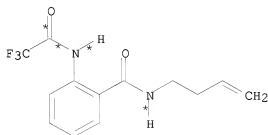
RX(31) RCT BF 112391-66-9
 RGT AW 302-01-2 N₂H₄
 PRO BG 112391-75-0
 SOL 64-17-5 EtOH

L3 ANSWER 181 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 107:134232 CASREACT
TITLE: Cycloadditions in syntheses. Part XXX. Photoaddition
 of 4(3H)-quinazolinone derivatives to olefins:
 effects of the 2-substituent
AUTHOR(S): Kaneko, Chikara; Kasai, Kouichi; Katagiri, Nobuya;
 Chiba, Takuo
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1986), 34(9),
 3672-81
 CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The photochem. behavior of 3-(3-butenyl)-4(3H)-quinazolinones I ($R = H, Cl, F_3C$) was examined in MeOH at a variety of wavelengths (254, 300, and 350 nm). The intramol. 2 + 2 photoadducts II ($n = 1, 2$) were obtained only when I ($R = F_3C$) and its higher methylene homolog were irradiated. Though the 2-unsubstituted quinazolinone I ($R = H$) was photostable I ($R = Cl$) afforded the cyclized product (III) via homolytic fission of the C-Cl bond. An enhancement of the photocycloaddn. reactivity of the C:N bond in the quinazolinone ring by introduction of a trifluoromethyl group was also demonstrated by the formation of the intermol. adducts from 2-trifluoromethyl-4(3H)-quinazolinone by irradiation in the presence of olefins. The reactions due to C-N bond fission of the azetidine ring in these adducts are also described. Rutecarpine (IV) was synthesized by irradiation of 2-chloro-3-[2-(indol-3-yl)ethyl]-4-(3H)-quinazolinone.

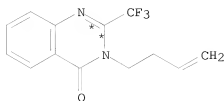
RX(8) OF 63 ...T ==> V...



T

(8) →

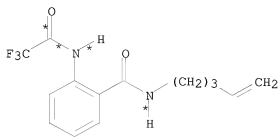
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V
YIELD 85%

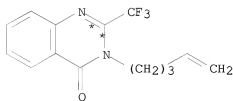
RX(8) RCT T 109071-12-7
PRO V 109071-13-8

RX(14) OF 63 ...AG ==> AH...



AG

(14)
→

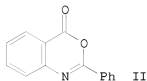
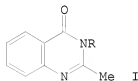


AH
YIELD 74%

RX(14) RCT AG 109071-16-1
PRO AH 109071-17-2

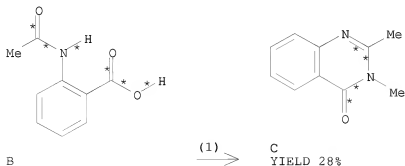
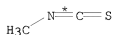
L3 ANSWER 182 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 107:77742 CASREACT
TITLE: One-pot synthesis of 2,3-disubstituted

AUTHOR(S): Ashare, Ram; Mukerjee, Arya K.
 CORPORATE SOURCE: Fac. Sci., Banaras Hindu Univ., Varanasi, 221 005, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1986), 25B(11), 1180-1
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



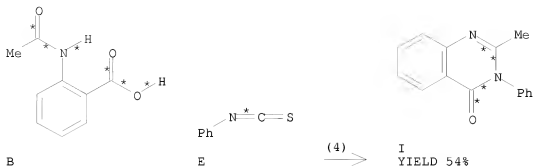
AB The condensation of N-acetylanthranilic acid with Me and Ph isothiocyanates affords the corresponding 3-substituted 2-methylquinazolin-4-ones I (R = Me, Ph), N-benzoylanthranilic acid reacts with these isothiocyanates to give 2-phenyl-3,1-benzoxazin-4-one II and 2-BzNHC6H4CONHPh resp.

RX(1) OF 4 A + B ==> C



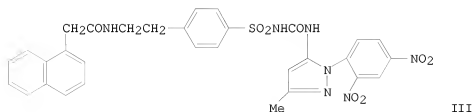
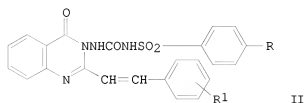
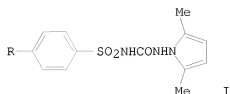
RX(1) RCT A 556-61-6, B 89-52-1
 RGT D 110-86-1 Pyridine
 PRO C 1769-25-1

RX(4) OF 4 B + E ==> I



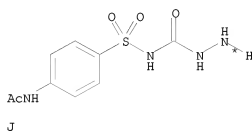
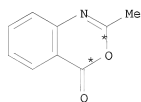
RX(4) RCT B 89-52-1, E 103-72-0
 RGT D 110-86-1 Pyridine
 PRO I 2385-23-1

L3 ANSWER 183 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 107:58968 CASREACT
 TITLE: Synthesis of some new substituted sulfonylureas as oral hypoglycemic agents
 AUTHOR(S): Husain, M. I.; Srivastava, V. P.
 CORPORATE SOURCE: Dep. Chem., Lucknow Univ., Lucknow, 226 007, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1986), 25B(9), 934-8
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



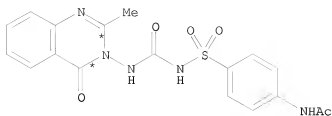
AB The title compds., e.g. I (R = H, Me, MeO, AcNH), II (R1 = 4-Me, 4-MeO, 4-Cl, 4-NO2) and III were prepared and their hypoglycemic activity evaluated. Some of these compds., when screened on albino rats at an oral dose of 250 mg/kg body weight, reduce the blood sugar to a significant extent.

RX(12) OF 107 ...N + J ==> V...



(12) →

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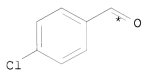


V

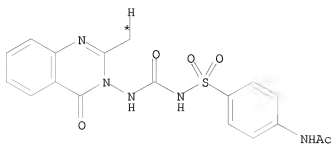
YIELD 62%

RX(12) RCT N 525-76-8, J 76983-56-7
PRO V 109274-28-4
SOL 110-86-1 Pyridine

RX(19) OF 107 ...AC + V ==> AG

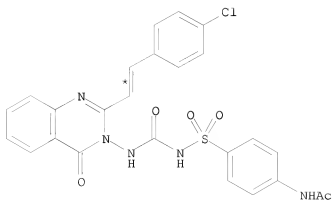


AC



V

(19)



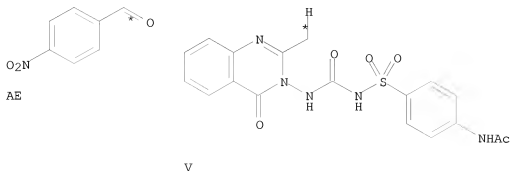
AG

YIELD 84%

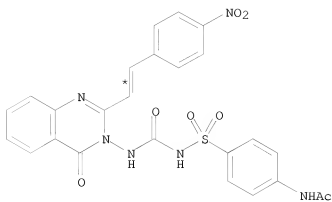
10/ 562,112

RX(19) RCT AC 104-88-1, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO AG 109274-46-6
 SOL 64-17-5 EtOH

RX(20) OF 107 ...AE + V ==> AH



(20)
→

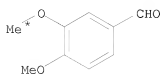


YIELD 76%

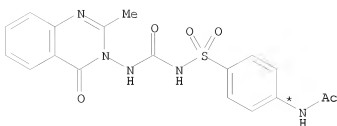
RX(20) RCT AE 555-16-8, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO AH 109274-47-7
 SOL 64-17-5 EtOH

RX(21) OF 107 ...AI + V ==> R...

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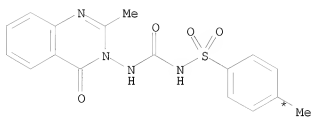


AI



V

(21)

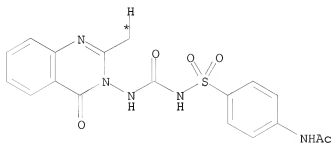


R

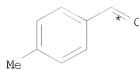
YIELD 82%

RX(21) RCT AI 120-14-9, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO R 109274-27-3
 SOL 64-17-5 EtOH

RX(23) OF 107 ...V + W ==> AK

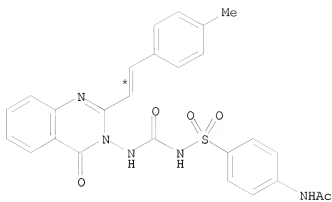


V



W

(23)

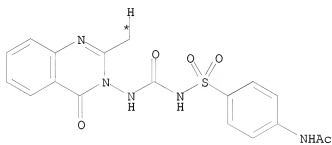


AK

YIELD 86%

RX(23) RCT V 109274-28-4, W 104-87-0
 RGT M 64-19-7 AcOH
 PRO AK 109274-44-4
 SOL 64-17-5 EtOH

RX(25) OF 107 ...V + Y ==> AM

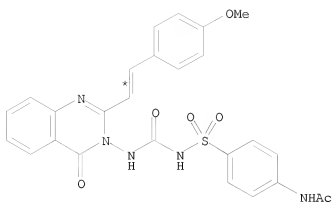


V



Y

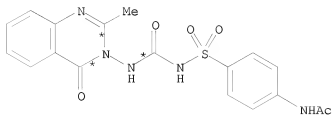
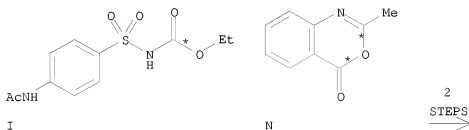
(25) →



AM
YIELD 76%

RX(25) RCT V 109274-28-4, Y 123-11-5
RGT M 64-19-7 AcOH
PRO AM 109274-45-5
SOL 64-17-5 EtOH

RX(45) OF 107 COMPOSED OF RX(4), RX(12)
RX(45) I + N ==> V



V
YIELD 62%

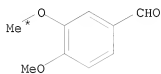
RX(4) RCT I 13945-59-0
RGT C 302-01-2 N2H4

10/ 562,112

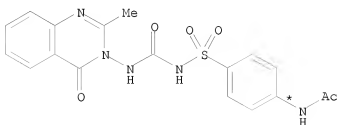
PRO J 76983-56-7
SOL 64-17-5 EtOH

RX(12) RCT N 525-76-8, J 76983-56-7
PRO V 109274-28-4
SOL 110-86-1 Pyridine

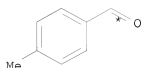
RX(56) OF 107 COMPOSED OF RX(21), RX(15)
RX(56) AI + V + W ==> AA



AI

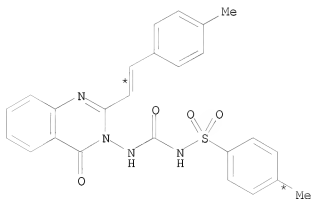


V



W

2
STEPS
→



AA

YIELD 54%

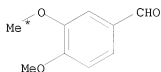
RX(21) RCT AI 120-14-9, V 109274-28-4
RGT M 64-19-7 AcOH
PRO R 109274-27-3

10/ 562,112

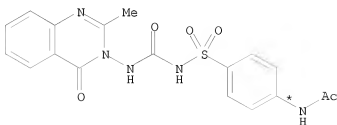
SOL 64-17-5 EtOH

RX(15) RCT W 104-87-0, R 109274-27-3
 RGT M 64-19-7 AcOH
 PRO AA 109274-34-2
 SOL 64-17-5 EtOH

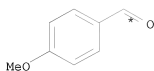
RX(57) OF 107 COMPOSED OF RX(21), RX(16)
 RX(57) AI + V + Y ==> AB



AI

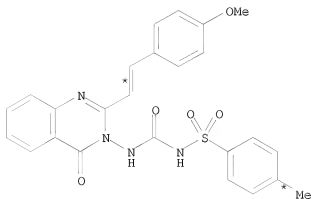


V



Y

2
 STEPS
 →



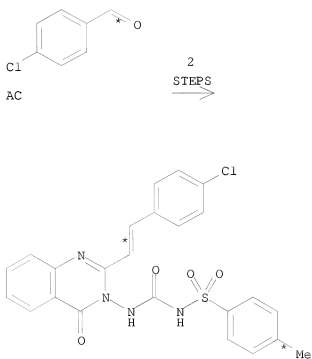
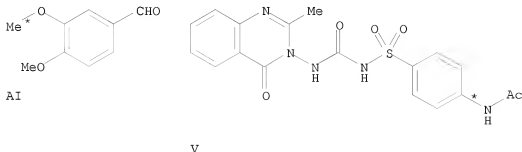
AB

YIELD 60%

RX(21) RCT AI 120-14-9, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO R 109274-27-3
 SOL 64-17-5 EtOH

RX(16) RCT Y 123-11-5, R 109274-27-3
 RGT M 64-19-7 AcOH
 PRO AB 109274-35-3
 SOL 64-17-5 EtOH

RX(58) OF 107 COMPOSED OF RX(21), RX(26)
 RX(58) AI + V + AC ==> AN



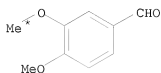
YIELD 68%

RX(21) RCT AI 120-14-9, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO R 109274-27-3
 SOL 64-17-5 EtOH

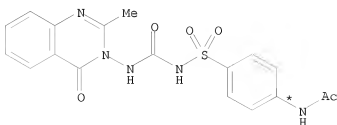
10/ 562,112

RX(26) RCT R 109274-27-3, AC 104-88-1
 RGT M 64-19-7 AcOH
 PRO AN 109274-36-4
 SOL 64-17-5 EtOH

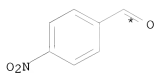
RX(59) OF 10⁷ COMPOSED OF RX(21), RX(29)
 RX(59) AI + V + AE ==> AQ



AI

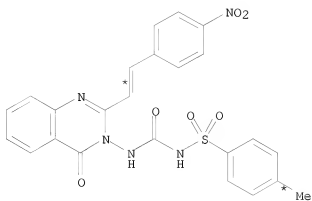


V



AE

2
 STEPS
 →



AQ

YIELD 72%

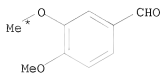
RX(21) RCT AI 120-14-9, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO R 109274-27-3
 SOL 64-17-5 EtOH

RX(29) RCT R 109274-27-3, AE 555-16-8

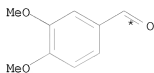
10/ 562,112

RGT M 64-19-7 AcOH
 PRO AQ 109274-37-5
 SOL 64-17-5 EtOH

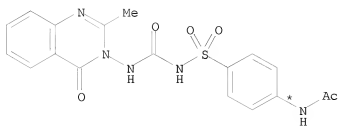
RX(60) OF 107 COMPOSED OF RX(21), RX(31)
 RX(60) 2 AI + V ==> AS



AI

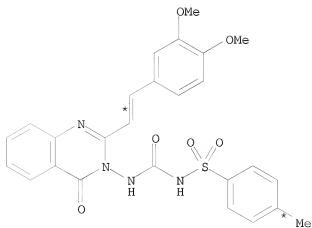


AI



V

2
 STEPS
 ➔



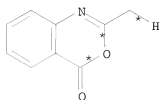
AS
 YIELD 58%

RX(21) RCT AI 120-14-9, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO R 109274-27-3
 SOL 64-17-5 EtOH

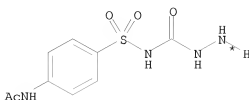
10/ 562,112

RX(31) RCT R 109274-27-3, AI 120-14-9
 RGT M 64-19-7 AcOH
 PRO AS 109274-38-6
 SOL 64-17-5 EtOH

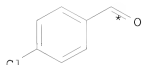
RX(66) OF 107 COMPOSED OF RX(12), RX(19)
 RX(66) N + J + AC ==> AG



N

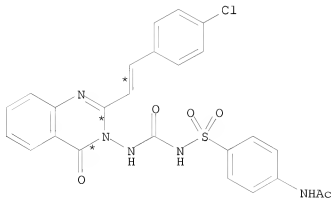


J



AC

2
 STEPS
 ➔



AG

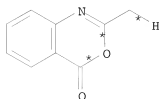
YIELD 84%

RX(12) RCT N 525-76-8, J 76983-56-7
 PRO V 109274-28-4
 SOL 110-86-1 Pyridine

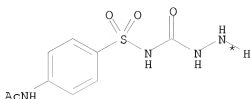
RX(19) RCT AC 104-88-1, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO AG 109274-46-6
 SOL 64-17-5 EtOH

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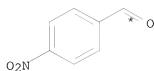
RX(67) OF 107 COMPOSED OF RX(12), RX(20)
 RX(67) N + J + AE ==> AH



N

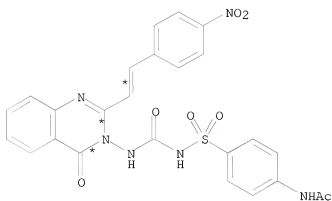


J



AE

2
 STEPS
 >



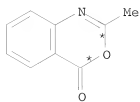
AH

YIELD 76%

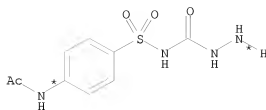
RX(12) RCT N 525-76-8, J 76983-56-7
 PRO V 109274-28-4
 SOL 110-86-1 Pyridine

RX(20) RCT AE 555-16-8, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO AH 109274-47-7
 SOL 64-17-5 EtOH

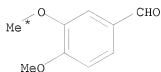
RX(68) OF 107 COMPOSED OF RX(12), RX(21)
 RX(68) N + J + AI ==> R



N

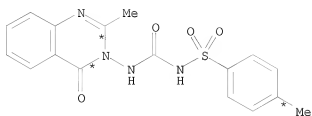


J



AI

2
STEPS
→



R

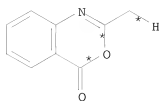
YIELD 82%

RX(12) RCT N 525-76-8, J 76983-56-7
PRO V 109274-28-4
SOL 110-86-1 Pyridine

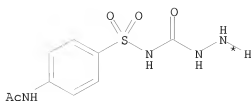
RX(21) RCT AI 120-14-9, V 109274-28-4
RGT M 64-19-7 AcOH
PRO R 109274-27-3
SOL 64-17-5 EtOH

RX(69) OF 107 COMPOSED OF RX(12), RX(23)

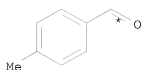
RX(69) N + J + W ==> AK



N

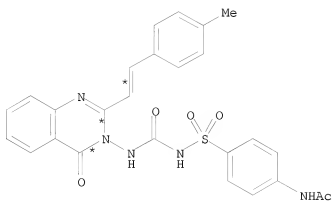


J



W

2
STEPS
→



AK

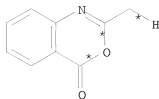
YIELD 86%

RX(12) RCT N 525-76-8, J 76983-56-7
PRO V 109274-28-4
SOL 110-86-1 Pyridine

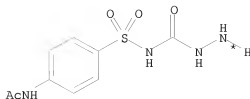
RX(23) RCT V 109274-28-4, W 104-87-0
RGT M 64-19-7 AcOH
PRO AK 109274-44-4
SOL 64-17-5 EtOH

RX(70) OF 107 COMPOSED OF RX(12), RX(25)
RX(70) N + J + Y ==> AM

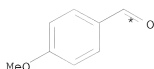
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N

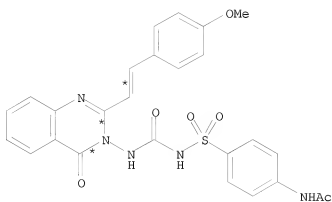


J



Y

2
STEPS
→



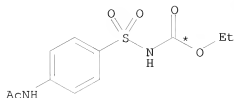
AM

YIELD 76%

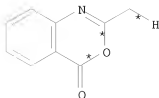
RX(12) RCT N 525-76-8, J 76983-56-7
PRO V 109274-28-4
SOL 110-86-1 Pyridine

RX(25) RCT V 109274-28-4, Y 123-11-5
RGT M 64-19-7 AcOH
PRO AM 109274-45-5
SOL 64-17-5 EtOH

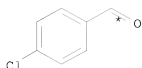
RX(90) OF 107 COMPOSED OF RX(4), RX(12), RX(19)
RX(90) I + N + AC ==> AG



I

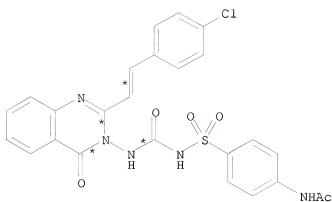


N



AC

3
STEPS
→



AG

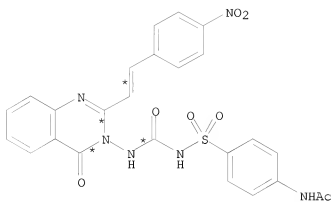
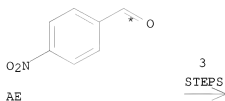
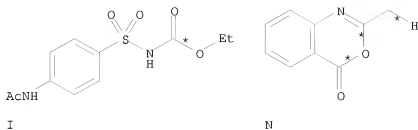
YIELD 84%

RX(4)	RCT	I 13945-59-0
	RGT	C 302-01-2 N2H4
	PRO	J 76983-56-7
	SOL	64-17-5 EtOH
RX(12)	RCT	N 525-76-8, J 76983-56-7
	PRO	V 109274-28-4
	SOL	110-86-1 Pyridine
RX(19)	RCT	AC 104-88-1, V 109274-28-4
	RGT	M 64-19-7 AcOH
	PRO	AG 109274-46-6
	SOL	64-17-5 EtOH

RX(91) OF 107 COMPOSED OF RX(4), RX(12), RX(20)

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RX(91) I + N + AE ==> AH

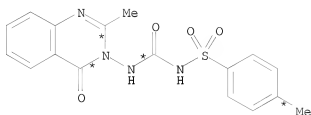
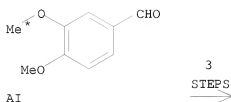
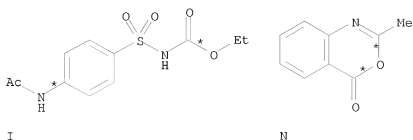


YIELD 76%

RX(4)	RCT	I 13945-59-0
	RGT	C 302-01-2 N2H4
	PRO	J 76983-56-7
	SOL	64-17-5 EtOH
RX(12)	RCT	N 525-76-8, J 76983-56-7
	PRO	V 109274-28-4
	SOL	110-86-1 Pyridine
RX(20)	RCT	AE 555-16-8, V 109274-28-4
	RGT	M 64-19-7 AcOH
	PRO	AH 109274-47-7
	SOL	64-17-5 EtOH

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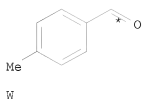
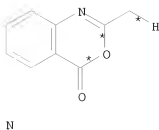
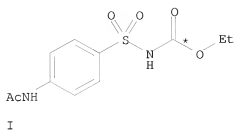
RX(92) OF 107 COMPOSED OF RX(4), RX(12), RX(21)
 RX(92) I + N + AI ==> R



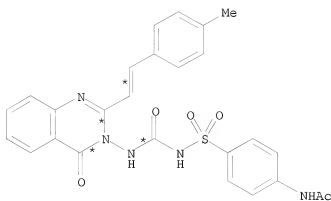
YIELD 82%

RX(4)	RCT	I 13945-59-0
	RGT	C 302-01-2 N2H4
	PRO	J 76983-56-7
	SOL	64-17-5 EtOH
RX(12)	RCT	N 525-76-8, J 76983-56-7
	PRO	V 109274-28-4
	SOL	110-86-1 Pyridine
RX(21)	RCT	AI 120-14-9, V 109274-28-4
	RGT	M 64-19-7 AcOH
	PRO	R 109274-27-3
	SOL	64-17-5 EtOH

RX(93) OF 107 COMPOSED OF RX(4), RX(12), RX(23)
 RX(93) I + N + W ==> AK



3
STEPS
→



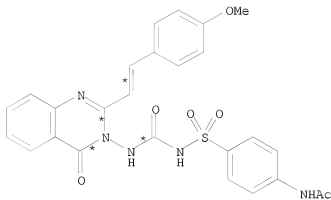
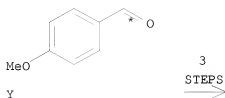
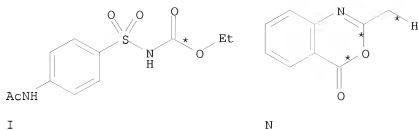
YIELD 86%

RX(4)	RCT	I 13945-59-0
	RGT	C 302-01-2 N2H4
	PRO	J 76983-56-7
	SOL	64-17-5 EtOH
RX(12)	RCT	N 525-76-8, J 76983-56-7
	PRO	V 109274-28-4
	SOL	110-86-1 Pyridine
RX(23)	RCT	V 109274-28-4, W 104-87-0
	RGT	M 64-19-7 AcOH
	PRO	AK 109274-44-4
	SOL	64-17-5 EtOH

RX(94) OF 107 COMPOSED OF RX(4), RX(12), RX(25)

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RX(94) I + N + Y ==> AM



YIELD 76%

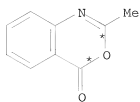
RX(4) RCT I 13945-59-0
RGT C 302-01-2 N2H4
PRO J 76983-56-7
SOL 64-17-5 EtOH

RX(12) RCT N 525-76-8, J 76983-56-7
PRO V 109274-28-4
SOL 110-86-1 Pyridine

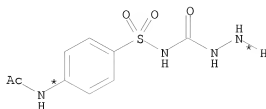
RX(25) RCT V 109274-28-4, Y 123-11-5
RGT M 64-19-7 AcOH
PRO AM 109274-45-5
SOL 64-17-5 EtOH

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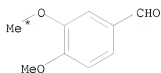
RX(95) OF 107 COMPOSED OF RX(12), RX(21), RX(15)
 RX(95) N + J + AI + W ==> AA



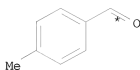
N



J

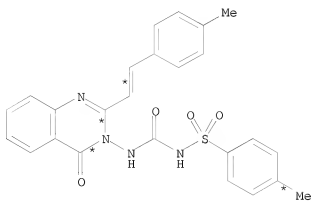


AI



W

3
STEPS
→



AA

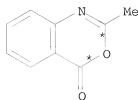
YIELD 54%

RX(12) RCT N 525-76-8, J 76983-56-7
 PRO V 109274-28-4
 SOL 110-86-1 Pyridine

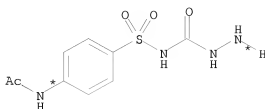
RX(21) RCT AI 120-14-9, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO R 109274-27-3
 SOL 64-17-5 EtOH

RX(15) RCT W 104-87-0, R 109274-27-3
 RGT M 64-19-7 AcOH
 PRO AA 109274-34-2
 SOL 64-17-5 EtOH

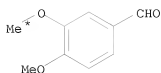
RX(96) OF 107 COMPOSED OF RX(12), RX(21), RX(16)
 RX(96) N + J + AI + Y ==> AB



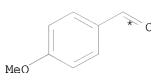
N



J

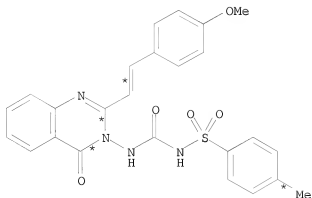


AI



Y

3
 STEPS
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AB

YIELD 60%

RX(12) RCT N 525-76-8, J 76983-56-7
 PRO V 109274-28-4
 SOL 110-86-1 Pyridine

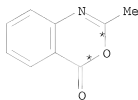
RX(21) RCT AI 120-14-9, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO R 109274-27-3
 SOL 64-17-5 EtOH

RX(16) RCT Y 123-11-5, R 109274-27-3
 RGT M 64-19-7 AcOH

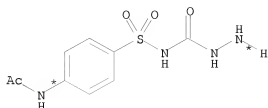
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PRO AB 109274-35-3
SOL 64-17-5 EtOH

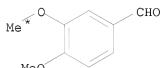
RX(97) OF 107 COMPOSED OF RX(12), RX(21), RX(26)
RX(97) N + J + AI + AC ==> AN



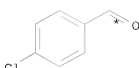
N



J

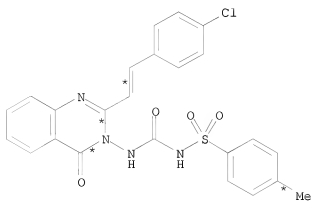


AI



AC

3
STEPS
→



AN

YIELD 68%

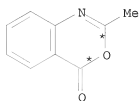
RX(12) RCT N 525-76-8, J 76983-56-7
PRO V 109274-28-4
SOL 110-86-1 Pyridine

RX(21) RCT AI 120-14-9, V 109274-28-4
RGT M 64-19-7 AcOH
PRO R 109274-27-3
SOL 64-17-5 EtOH

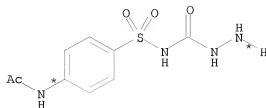
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RX(26) RCT R 109274-27-3, AC 104-88-1
 RGT M 64-19-7 AcOH
 PRO AN 109274-36-4
 SOL 64-17-5 EtOH

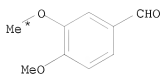
RX(98) OF 10⁷ COMPOSED OF RX(12), RX(21), RX(29)
 RX(98) N + J + AI + AE ==> AQ



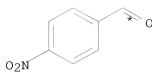
N



J

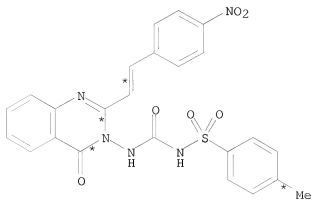


AI



AE

3
 STEPS
 →



AQ

YIELD 72%

RX(12) RCT N 525-76-8, J 76983-56-7
 PRO V 109274-28-4
 SOL 110-86-1 Pyridine

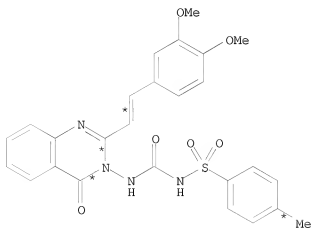
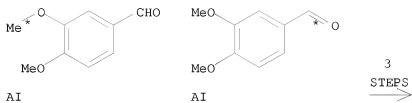
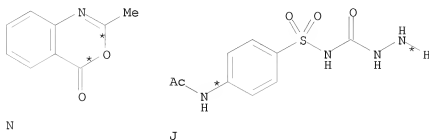
RX(21) RCT AI 120-14-9, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO R 109274-27-3

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SOL 64-17-5 EtOH

RX(29) RCT R 109274-27-3, AE 555-16-8
RGT M 64-19-7 AcOH
PRO AQ 109274-37-5
SOL 64-17-5 EtOH

RX(99) OF 107 COMPOSED OF RX(12), RX(21), RX(31)
RX(99) N + J + 2 AI ==> AS



AS
YIELD 58%

RX(12) RCT N 525-76-8, J 76983-56-7
PRO V 109274-28-4
SOL 110-86-1 Pyridine

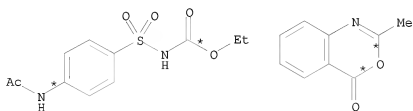
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RX(21) RCT AI 120-14-9, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO R 109274-27-3
 SOL 64-17-5 EtOH

RX(31) RCT R 109274-27-3, AI 120-14-9
 RGT M 64-19-7 AcOH
 PRO AS 109274-38-6
 SOL 64-17-5 EtOH

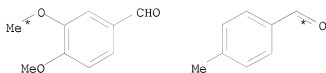
RX(100) OF 107 COMPOSED OF RX(4), RX(12), RX(21), RX(15)

RX(100) I + N + AI + W ==> AA



I

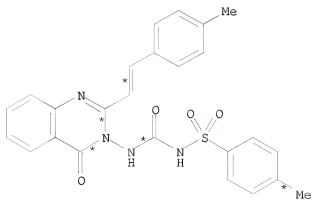
N



AI

W

4
STEPS
→



AA

YIELD 54%

RX(4) RCT I 13945-59-0

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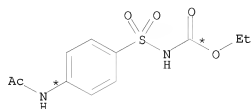
RGT C 302-01-2 N2H4
 PRO J 76983-56-7
 SOL 64-17-5 EtOH

RX(12) RCT N 525-76-8, J 76983-56-7
 PRO V 109274-28-4
 SOL 110-86-1 Pyridine

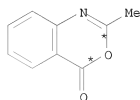
RX(21) RCT AI 120-14-9, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO R 109274-27-3
 SOL 64-17-5 EtOH

RX(15) RCT W 104-87-0, R 109274-27-3
 RGT M 64-19-7 AcOH
 PRO AA 109274-34-2
 SOL 64-17-5 EtOH

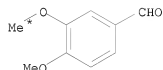
RX(101) OF 107 COMPOSED OF RX(4), RX(12), RX(21), RX(16)
 RX(101) I + N + AI + Y ==> AB



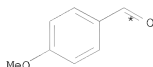
I



N

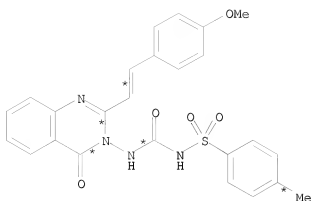


AI



Y

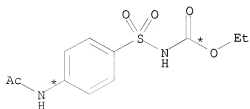
4
 STEPS
 →



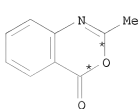
AB
YIELD 60%

RX(4)	RCT	I 13945-59-0
	RGT	C 302-01-2 N2H4
	PRO	J 76983-56-7
	SOL	64-17-5 EtOH
RX(12)	RCT	N 525-76-8, J 76983-56-7
	PRO	V 109274-28-4
	SOL	110-86-1 Pyridine
RX(21)	RCT	AI 120-14-9, V 109274-28-4
	RGT	M 64-19-7 AcOH
	PRO	R 109274-27-3
	SOL	64-17-5 EtOH
RX(16)	RCT	Y 123-11-5, R 109274-27-3
	RGT	M 64-19-7 AcOH
	PRO	AB 109274-35-3
	SOL	64-17-5 EtOH

RX(102) OF 107 COMPOSED OF RX(4), RX(12), RX(21), RX(26)
RX(102) I + N + AI + AC ==> AN

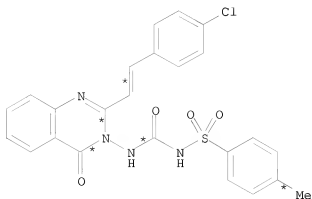
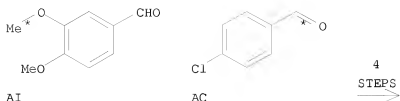


I



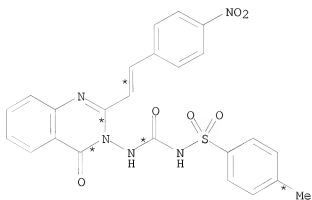
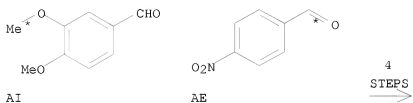
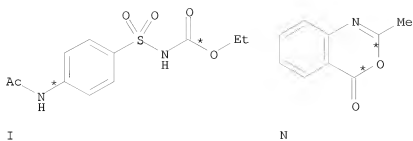
N

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AN
YIELD 68%

RX(4)	RCT	I 13945-59-0
	RGT	C 302-01-2 N2H4
	PRO	J 76983-56-7
	SOL	64-17-5 EtOH
RX(12)	RCT	N 525-76-8, J 76983-56-7
	PRO	V 109274-28-4
	SOL	110-86-1 Pyridine
RX(21)	RCT	AI 120-14-9, V 109274-28-4
	RGT	M 64-19-7 AcOH
	PRO	R 109274-27-3
	SOL	64-17-5 EtOH
RX(26)	RCT	R 109274-27-3, AC 104-88-1
	RGT	M 64-19-7 AcOH
	PRO	AN 109274-36-4
	SOL	64-17-5 EtOH
RX(103) OF 107 COMPOSED OF RX(4), RX(12), RX(21), RX(29)		
RX(103)	I + N + AI + AE	==> AQ



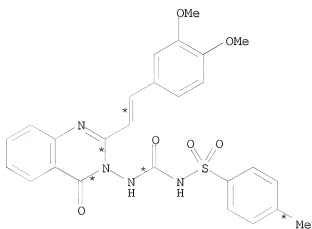
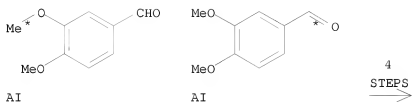
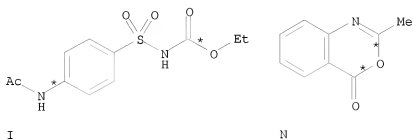
YIELD 72%

RX(4)	RCT	I 13945-59-0
	RGT	C 302-01-2 N2H4
	PRO	J 76983-56-7
	SOL	64-17-5 EtOH
RX(12)	RCT	N 525-76-8, J 76983-56-7
	PRO	V 109274-28-4
	SOL	110-86-1 Pyridine
RX(21)	RCT	AI 120-14-9, V 109274-28-4
	RGT	M 64-19-7 AcOH
	PRO	R 109274-27-3
	SOL	64-17-5 EtOH

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RX(29) RCT R 109274-27-3, AE 555-16-8
 RGT M 64-19-7 AcOH
 PRO AQ 109274-37-5
 SOL 64-17-5 EtOH

RX(104) OF 107 COMPOSED OF RX(4), RX(12), RX(21), RX(31)
 RX(104) I + N + 2 AI ==> AS



YIELD 58%

RX(4) RCT I 13945-59-0
 RGT C 302-01-2 N2H4
 PRO J 76983-56-7
 SOL 64-17-5 EtOH

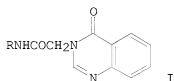
RX(12) RCT N 525-76-8, J 76983-56-7
 PRO V 109274-28-4
 SOL 110-86-1 Pyridine

RX(21) RCT AI 120-14-9, V 109274-28-4
 RGT M 64-19-7 AcOH
 PRO R 109274-27-3
 SOL 64-17-5 EtOH

RX(31) RCT R 109274-27-3, AI 120-14-9
 RGT M 64-19-7 AcOH
 PRO AS 109274-38-6
 SOL 64-17-5 EtOH

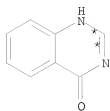
L3 ANSWER 184 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 106:196363 CASREACT
 TITLE: Monoamine oxidase and succinate dehydrogenase
 inhibitory and anticonvulsant activities of some
 3-(N-arylcarbamoylmethyl)-4-quinazolones
 AUTHOR(S): Saksena, R. K.; Yasmeen, Rana, Ms.
 CORPORATE SOURCE: D.A.V. Coll., Kanpur Univ., Kanpur, 208 001, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (1986),
 25B(4), 438-40
 CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

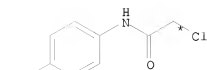


AB 3-(N-Arylcarbamoylmethyl)-4-quinazolones I (R = Ph, substituted phenyl)
 (11 compds.) were prepared from RNHCOCH₂Cl and 4-quinazolone. I have ALD50
 values from 500-1000 mg/kg and inhibit rat brain monoamine oxidase
 (30-65%) and succinate dehydrogenase (10-80%) in vitro at a concentration of 5
 + 10-4 M and provide 30-50% protection against
 pentylenetetrazole-induced convulsions in mice.

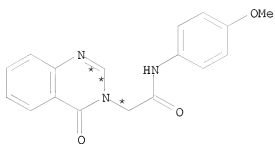
RX(1) OF 33 ...A + B ==> C



A



G

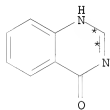
(3) \Rightarrow 

H

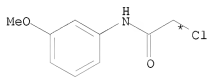
YIELD 65%

RX(3) RCT A 491-36-1, G 22303-36-2
 PRO H 108086-40-4
 SOL 110-86-1 Pyridine

RX(4) OF 33 ...A + I ==> J

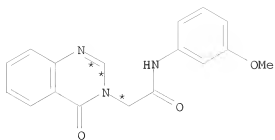


A



I

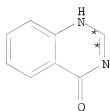
(4) \Rightarrow



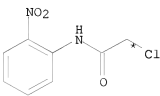
J
YIELD 75%

RX(4) RCT A 491-36-1, I 17641-08-6
PRO J 108086-41-5
SOL 110-86-1 Pyridine

RX(5) OF 33 ...A + K ==> L

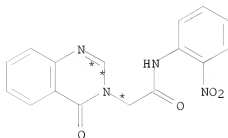


A



K

(5) \longrightarrow

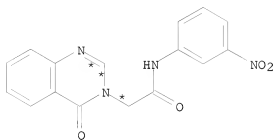
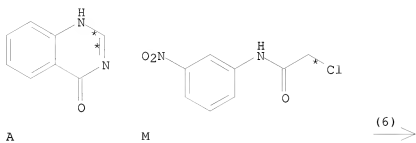


L
YIELD 70%

RX(5) RCT A 491-36-1, K 10147-70-3
PRO L 108086-42-6
SOL 110-86-1 Pyridine

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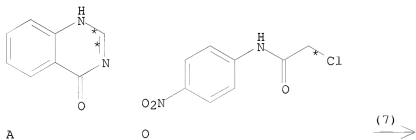
RX(6) OF 33 ...A + M ==> N

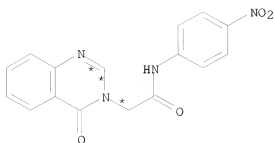


N
YIELD 60%

RX(6) RCT A 491-36-1, M 10147-71-4
 PRO N 108086-43-7
 SOL 110-86-1 Pyridine

RX(7) OF 33 ...A + O ==> P

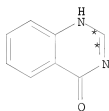




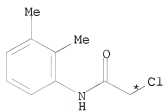
P
YIELD 65%

RX(7) RCT A 491-36-1, O 17329-87-2
 PRO P 108086-44-8
 SOL 110-86-1 Pyridine

RX(8) OF 33 ...A + Q ==> R

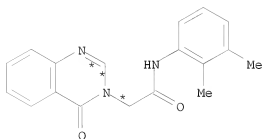


A



Q

(8) \longrightarrow

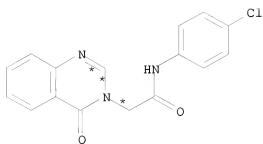
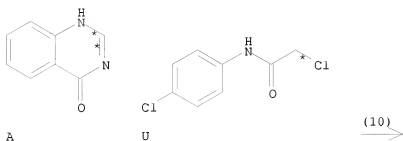


R
YIELD 68%

RX(8) RCT A 491-36-1, Q 2564-07-0
 PRO R 108086-45-9
 SOL 110-86-1 Pyridine

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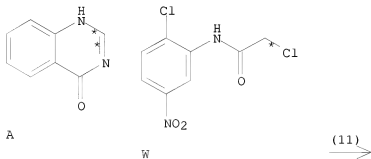
RX(10) OF 33 ...A + U ==> V

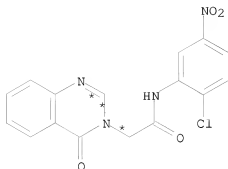


V
YIELD 70%

RX(10) RCT A 491-36-1, U 3289-75-6
 PRO V 108086-47-1
 SOL 110-86-1 Pyridine

RX(11) OF 33 ...A + W ==> X

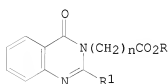




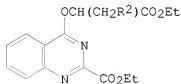
X
YIELD 55%

RX(11) RCT A 491-36-1, W 108086-37-9
PRO X 108086-48-2
SOL 110-86-1 Pyridine

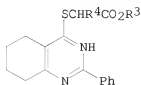
L3 ANSWER 185 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 106:138387 CASREACT
TITLE: Quinazolinecarboxylic acid. Synthesis of
alkyl[2-(ethoxycarbonyl)-3,4-dihydro-4-oxoquinazolin-3-
yl]-, [2-(ethoxycarbonyl)quinazolin-4-yl]oxy- and
(5,6,7,8-tetrahydro-2-phenylquinazolin-4-
ylthio)alkanoates
AUTHOR(S): Suesse, Manfred; Adler, Frank; John, Siegfried
CORPORATE SOURCE: Inst. Biochem. Pflanzen Halle, Dtsch. Akad. Wiss.,
Halle/Saale, DDR-4010, Ger. Dem. Rep.
SOURCE: Helvetica Chimica Acta (1986), 69(5), 1017-24
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



II



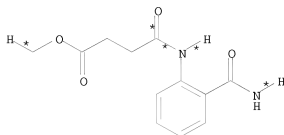
IV



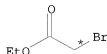
V

AB Cyclization of 2-H₂NC₆H₄CONH(CH₂)_nCO₂Et (I, n = 2, 3) with EtO₂CCO₂Et gave quinazolines II (R = Et, R₁ = CO₂Et), whereas, condensation of I (n = 1) with ClCOCO₂Et gave a mixture of 2-EtO₂CCONHC₆H₄CONHCH₂CO₂Et and II (n = 1, R = Et, R₁ = CO₂Et). Cyclization of 2-H₂NC₆H₄CONH₂ (III) with EtO₂CCO₂Et followed by condensation with BrCH₂CO₂R (R = Me, Et) gave II (n = 1, R = Me, Et, R₁ = CO₂Et), whereas, cyclization of III with EtO₂CCO₂Et followed by condensation with R₂CH₂CHBrCO₂Et (R₂ = H, Me) gave quinazoline esters IV. Condensation of III with ClCOCH₂CH₂CO₂Me gave 2-H₂NCOC₆H₄NHCOCH₂CH₂CO₂Me which was cyclized with BrCH₂CO₂Et to give II (n = 1, R = Et, R₁ = CH₂CH₂CO₂CH₂CO₂Et). Quinazoline thioethers V (R₃ = Me, Et, R₄ = H, Et, CHMe₂) were prepared by aminolysis of 5,6,7,8-tetrahydro-1,3-benzoxazine-4(3H)-thione followed by condensation with BrCHR₄CO₂R₃.

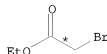
RX(11) OF 27 ...AC + 2 AD ==> AE



AC

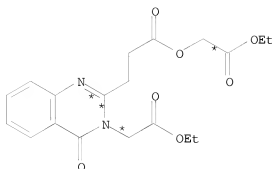


AD



AD

(11) →



AE
YIELD 22%

RX(11) RCT AC 105234-41-1

STAGE(1)

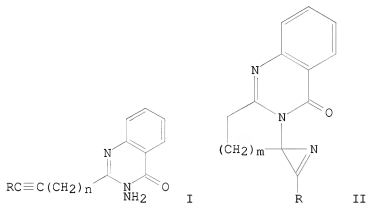
RGT P 7646-69-7 NaH

SOL 67-68-5 DMSO

STAGE(2)
RCT AD 105-36-2

PRO AE 105234-42-2

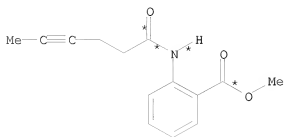
L3 ANSWER 186 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 106:138380 CASREACT
 TITLE: Intramolecular reactions of N-nitrenes with alkynes:
 conformational anchoring in spiro-fused 2H-azirines
 AUTHOR(S): Atkinson, Robert S.; Grimshire, Michael J.
 CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999)
 (1986), (7), 1215-24
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Oxidation of aminoquinazolinones, e.g., I ($n = 2$, $R = H$, Me; $n = 3$, $R = H$) with $Pb(OAc)_4$ in CH_2Cl_2 results in the intramol. addition of the N-nitrene to the triple bond in each case and azirines II ($m = 1$, $R = H$, Me; $m = 2$, $R = H$) are isolated. An x-ray crystal structure determination of II ($m = 1$, $R = H$) reveals a remarkable deformation of bond angles at the spiro center and this feature appears to be common to all azirines. The five membered ring in II ($m = 1$) has the envelope conformation and the six-membered ring in II ($m = 2$) has the twist-boat conformation; a possible explanation for this conformational anchoring is offered.

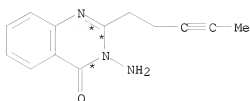
RX(7) OF 260 ...P ==> Q...

10/ 562,112



P

(7) \longrightarrow

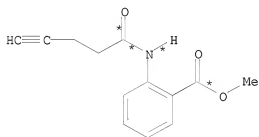


Q

YIELD 90%

RX(7) RCT P 107428-13-7
 RGT R 302-01-2 N2H4
 PRO Q 98750-79-9
 SOL 64-17-5 EtOH

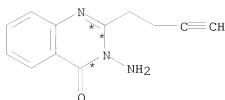
RX(8) OF 260 ...S ==> T...



S

(8) \longrightarrow

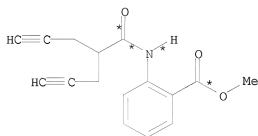
10/ 562,112



T
YIELD 46%

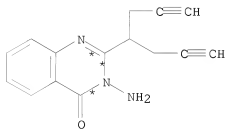
RX(8) RCT S 107428-12-6
 RGT R 302-01-2 N2H4
 PRO T 98750-77-7
 SOL 64-17-5 EtOH

RX(14) OF 260 ...AD ==> AA...



AD

(14)
→

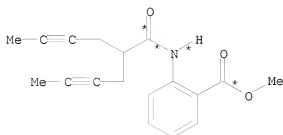


AA
YIELD 63%

RX(14) RCT AD 107428-15-9
 RGT R 302-01-2 N2H4
 PRO AA 98750-78-8
 SOL 64-17-5 EtOH
 NTE Product varies with reactors tiime

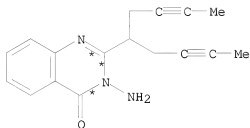
10/ 562,112

RX(16) OF 260 ...AF ==> AG...



AF

(16) 

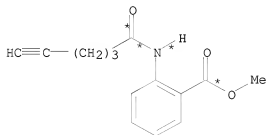


AG

YIELD 59%

RX(16) RCT AF 107428-16-0
 RGT R 302-01-2 N2H4
 PRO AG 107428-08-0
 SOL 64-17-5 EtOH

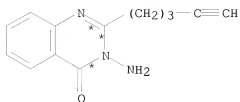
RX(18) OF 260 ...AI ==> AJ...



AI

(18) 

10/ 562,112

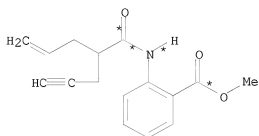


AJ

YIELD 70%

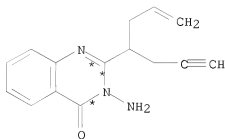
RX(18)	RCT	AI 107428-14-8
	RGT	R 302-01-2 N2H4
	PRO	AJ 98750-87-9
	SOL	64-17-5 EtOH

RX(39) OF 260 ...BJ ==> BK...



BJ

(39) →



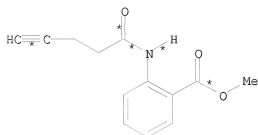
BK

RX(39)	RCT	BJ 107428-21-7
	RGT	R 302-01-2 N2H4
	PRO	BK 107428-22-8
	SOL	64-17-5 EtOH

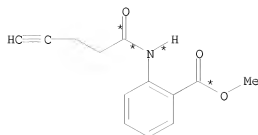
RX(55) OF 260 COMPOSED OF RX(8), RX(10)

10/ 562,112

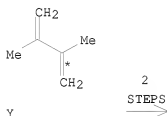
RX(55) 2 S + Y ==> V + Z



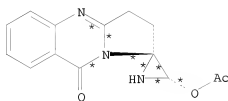
S



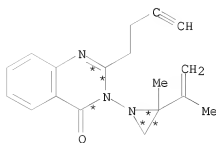
S



Y



V



Z

RX(8) RCT S 107428-12-6
RGT R 302-01-2 N2H4
PRO T 98750-77-7
SOL 64-17-5 EtOH

RX(10) RCT T 98750-77-7

STAGE(1)

RGT W 546-67-8 Pb(OAc)4
SOL 75-09-2 CH2Cl2

STAGE(2)

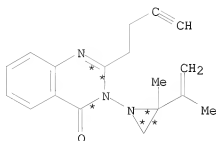
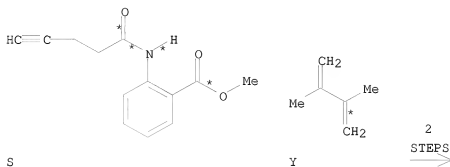
RCT Y 513-81-5

PRO V 98750-85-7, Z 107428-11-5

10/ 562,112

RX(56) OF 260 COMPOSED OF RX(8), RX(11)

RX(56) S + Y ==> Z



Z

RX(8) RCT S 107428-12-6
RGT R 302-01-2 N2H4
PRO T 98750-77-7
SOL 64-17-5 EtOH

RX(11) RCT Y 513-81-5, T 98750-77-7
RGT W 546-67-8 Pb(OAc)4
PRO Z 107428-11-5
SOL 75-09-2 CH2Cl2

L3 ANSWER 187 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 106:102196 CASREACT

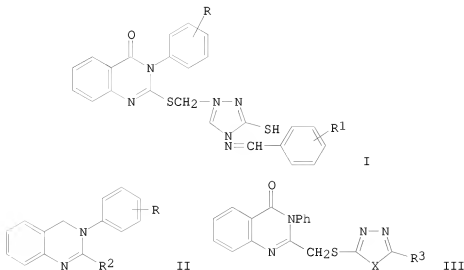
TITLE: Synthesis of certain new sulfur-containing
quinazolinone derivatives likely to possess CNS
depressant action

AUTHOR(S): El-Feky, S. A.; Al-Ashmawi, M. I.; Hazzaa, A. A. B.;
El-Fattah, B. Abd

CORPORATE SOURCE: Fac. Pharm., Zagazig Univ., Egypt
SOURCE: Egyptian Journal of Pharmaceutical Sciences (1985),
Volume Date 1983, 24(1-4), 39-47
CODEN: EJPSBZ; ISSN: 0301-5068

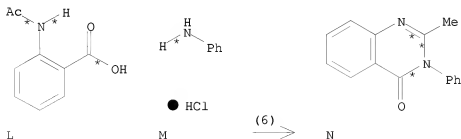
DOCUMENT TYPE:
LANGUAGE:
GI

Journal
English



AB Quinazolines I (R = H, 2-Me, 4-Me; R₁ = H, 4-Cl, 3-NO₂, 4-NO₂, 4-MeO, 2-OH, 4-OH) were prepared from amides II (R₂ = SCH₂CONHNH₂), by dithiocarboxylation followed by cyclocondensation with N₂H₄ and condensation of R₁C₆H₄CHO. Condensation of II (R₁ = H, R₂ = CH₂Br) with triazoles and oxadiazoles yielded compds. III (X = O, NNH₂; by dithiocarboxylation followed by cyclocondensation with N₂H₄ and condensation with R₁C₆H₄CHO. Condensation of II (R₁ = H, R₂ = CH₂Br) with triazoles and oxadiazoles yielded compds. III (X = O, NNH₂; R₃ = Ph, 3-pyridyl, 4-pyridyl, 4-ClC₆H₄OCH₂, Z = ClC₆H₄OCH₂). The anticonvulsant activity of several I-III were tested (no data).

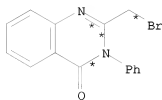
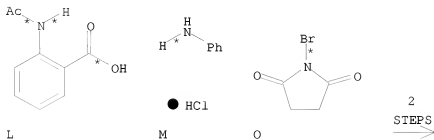
RX(6) OF 169 ...L + M ==> N...



RX(6) RCT L 89-52-1, M 142-04-1
PRO N 2385-23-1

10/ 562,112

RX(46) OF 169 COMPOSED OF RX(6), RX(7)
 RX(46) L + M + O ==> P

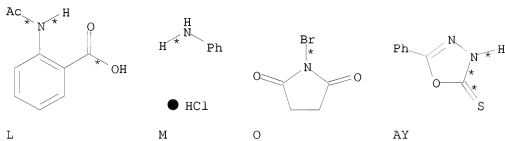


P

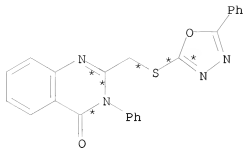
RX(6) RCT L 89-52-1, M 142-04-1
 PRO N 2385-23-1

RX(7) RCT N 2385-23-1, O 128-08-5
 PRO P 19062-58-9

RX(85) OF 169 COMPOSED OF RX(6), RX(7), RX(32)
 RX(85) L + M + O + AY ==> AZ



3
 STEPS

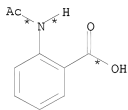
AZ

RX(6) RCT L 89-52-1, M 142-04-1
PRO N 2385-23-1

RX(7) RCT N 2385-23-1, O 128-08-5
PRO P 19062-58-9

RX(32) RCT P 19062-58-9, AY 3004-42-0
PRO AZ 105491-93-8
SOL 67-64-1 Me2CO

RX(86) OF 169 COMPOSED OF RX(6), RX(7), RX(33)
RX(86) L + M + O + BB ==> BC

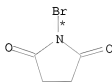


L

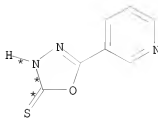


M

● HCl

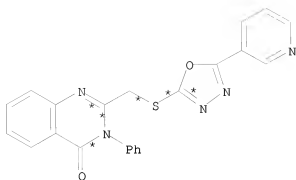


O



BB

3
STEPS
→



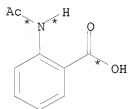
BC

RX(6) RCT L 89-52-1, M 142-04-1
PRO N 2385-23-1

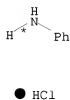
RX(7) RCT N 2385-23-1, O 128-08-5
PRO P 19062-58-9

RX(33) RCT P 19062-58-9, BB 3690-46-8
PRO BC 105491-94-9
SOL 67-64-1 Me2CO

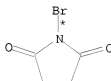
RX(87) OF 169 COMPOSED OF RX(6), RX(7), RX(34)
RX(87) L + M + O + BD ==> BE



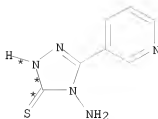
L



M

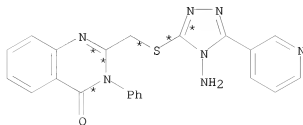


O



BD

3
STEPS
=>



BE

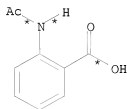
10/ 562,112

RX(6) RCT L 89-52-1, M 142-04-1
 PRO N 2385-23-1

RX(7) RCT N 2385-23-1, O 128-08-5
 PRO P 19062-58-9

RX(34) RCT P 19062-58-9, BD 78027-00-6
 PRO BE 105491-97-2
 SOL 67-64-1 Me2CO

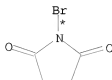
RX(88) OF 169 COMPOSED OF RX(6), RX(7), RX(35)
 RX(88) L + M + O + BF ==> BG



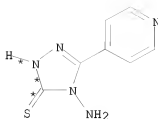
L



M

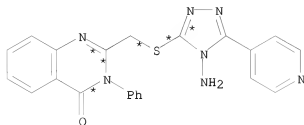


O



BF

3
 STEPS
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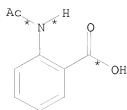
BG

RX(6) RCT L 89-52-1, M 142-04-1
 PRO N 2385-23-1

RX(7) RCT N 2385-23-1, O 128-08-5
 PRO P 19062-58-9

RX(35) RCT P 19062-58-9, BF 36209-51-5
 PRO BG 105491-98-3
 SOL 67-64-1 Me2CO

RX(89) OF 169 COMPOSED OF RX(6), RX(7), RX(36)
 RX(89) L + M + O + BH ==> BI

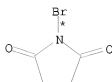


L

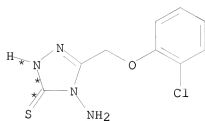


● HCl

M

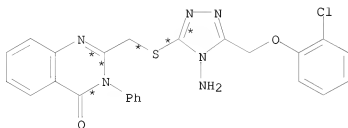


O



BH

3
STEPS
→



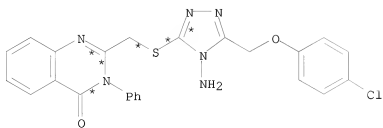
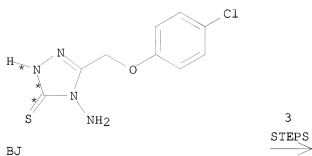
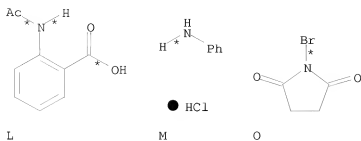
BI

RX(6) RCT L 89-52-1, M 142-04-1
PRO N 2385-23-1

RX(7) RCT N 2385-23-1, O 128-08-5
PRO P 19062-58-9

RX(36) RCT P 19062-58-9, BH 4413-42-7
PRO BI 105491-99-4
SOL 67-64-1 Me2CO

RX(90) OF 169 COMPOSED OF RX(6), RX(7), RX(37)
RX(90) L + M + O + BJ ==> BK



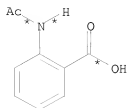
BK

RX(6) RCT L 89-52-1, M 142-04-1
 PRO N 2385-23-1

RX(7) RCT N 2385-23-1, O 128-08-5
 PRO P 19062-58-9

RX(37) RCT P 19062-58-9, BJ 4413-43-8
 PRO BK 105492-00-0
 SOL 67-64-1 Me2CO

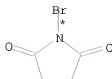
RX(91) OF 169 COMPOSED OF RX(6), RX(7), RX(40)
 RX(91) L + M + O + BM ==> BN



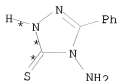
L



M

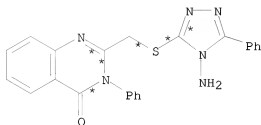


O



BM

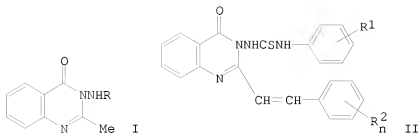
3
STEPS
→



BN

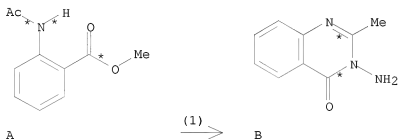
RX(6)	RCT	L 89-52-1, M 142-04-1
	PRO	N 2385-23-1
RX(7)	RCT	N 2385-23-1, O 128-08-5
	PRO	P 19062-58-9
RX(40)	RCT	P 19062-58-9, BM 22706-11-2
	PRO	BN 105491-96-1
	SOL	67-64-1 Me2CO

L3	ANSWER 188 OF 258	CASREACT	COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:		106:50150	CASREACT
TITLE:		Possible antiParkinsonian compounds. Synthesis of 2-styryl-3-arylthiouryl-3,4-dihydro-4-oxoquinazolines	
AUTHOR(S):		Pandey, V. K.	
CORPORATE SOURCE:		Dep. Chem., Univ. Lucknow, Lucknow, 226 001, India	
SOURCE:		Current Science (1986), 55(5), 243-6	
		CODEN: CUSCAM; ISSN: 0011-3891	
DOCUMENT TYPE:		Journal	
LANGUAGE:		English	
GI			



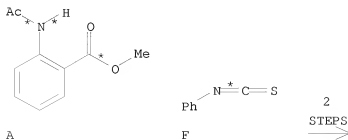
AB o-AcNHC6H4CO2Me, obtained by acetylation of o-H2NC6H4CO2Me, was cyclized with N2H4.H2O to give quinazolinone I (R = H), which was condensed with R1C6H4NCS to give thioureido derivs. I (R = CSNHC6H4R1), which on condensation with R2nC6H5-nCHO gave 6 title derivs. II [R1 = H, R2n = o-OMe (III), o-OH; R1 = 4-Me, R2n = o-Me, o-OH; R1 = 3-Me, R2n = 2-MeO-5-OH, o-OH]. None of II exhibited any significant antioxotremorine activity in mice at an i.p. dose of 100 mg/kg. III exhibited considerable central nervous system depressant activity.

RX(1) OF 36 ...A ==> B...

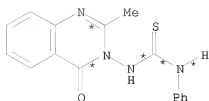


RX(1) RCT A 2719-08-6
 RGT C 302-01-2 N2H4
 PRO B 1898-06-2

RX(12) OF 36 COMPOSED OF RX(1), RX(3)
 RX(12) A + F ==> G



10/ 562,112



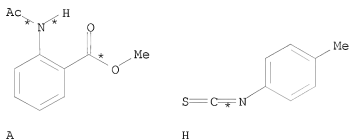
G

YIELD 50%

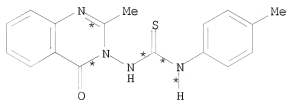
RX(1) RCT A 2719-08-6
RGT C 302-01-2 N2H4
PRO B 1898-06-2

RX(3) RCT B 1898-06-2, F 103-72-0
PRO G 62495-71-0

RX(13) OF 36 COMPOSED OF RX(1), RX(4)
RX(13) A + H ==> I



2
STEPS
→



I

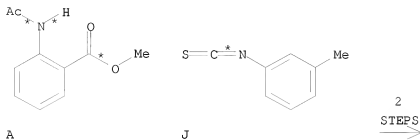
YIELD 50%

RX(1) RCT A 2719-08-6
RGT C 302-01-2 N2H4
PRO B 1898-06-2

RX(4) RCT B 1898-06-2, H 622-59-3
PRO I 87200-42-8

RX(14) OF 36 COMPOSED OF RX(1), RX(5)

RX(14) A + J ==> K

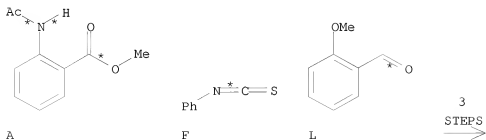
K
YIELD 50%

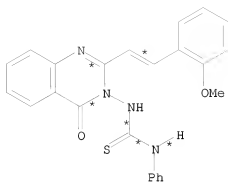
RX(1) RCT A 2719-08-6
RGT C 302-01-2 N2H4
PRO B 1898-06-2

RX(5) RCT B 1898-06-2, J 621-30-7
PRO K 105886-56-4

RX(22) OF 36 COMPOSED OF RX(1), RX(3), RX(6)

RX(22) A + F + L ==> M





M

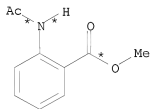
YIELD 30%

RX(1) RCT A 2719-08-6
 RGT C 302-01-2 N2H4
 PRO B 1898-06-2

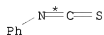
RX(3) RCT B 1898-06-2, F 103-72-0
 PRO G 62495-71-0

RX(6) RCT G 62495-71-0, L 135-02-4
 PRO M 105886-57-5

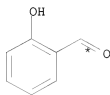
RX(23) OF 36 COMPOSED OF RX(1), RX(3), RX(7)
 RX(23) A + F + N ==> O



A

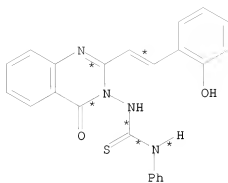


F



N

3
 STEPS
 →



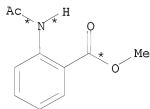
O
YIELD 30%

RX(1) RCT A 2719-08-6
RGT C 302-01-2 N2H4
PRO B 1898-06-2

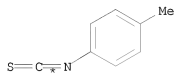
RX(3) RCT B 1898-06-2, F 103-72-0
PRO G 62495-71-0

RX(7) RCT G 62495-71-0, N 90-02-8
PRO O 105886-58-6

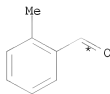
RX(24) OF 36 COMPOSED OF RX(1), RX(4), RX(8)
RX(24) A + H + P ==> Q



A

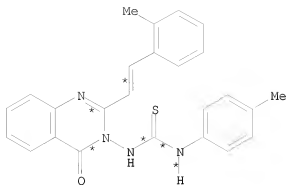


H



P

3
STEPS
→



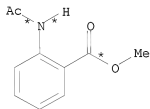
Q
YIELD 90%

RX(1) RCT A 2719-08-6
RGT C 302-01-2 N2H4
PRO B 1898-06-2

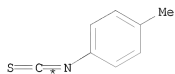
RX(4) RCT B 1898-06-2, H 622-59-3
PRO I 87200-42-8

RX(8) RCT I 87200-42-8, P 529-20-4
PRO Q 105886-59-7

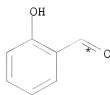
RX(25) OF 36 COMPOSED OF RX(1), RX(4), RX(9)
RX(25) A + H + N ==> R



A

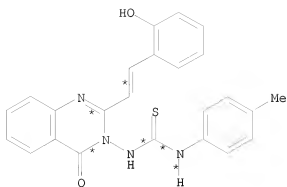


H



N

3
STEPS
→



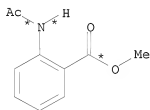
R
YIELD 30%

RX(1) RCT A 2719-08-6
RGT C 302-01-2 N2H4
PRO B 1898-06-2

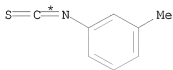
RX(4) RCT B 1898-06-2, H 622-59-3
PRO I 87200-42-8

RX(9) RCT I 87200-42-8, N 90-02-8
PRO R 105886-60-0

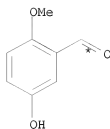
RX(26) OF 36 COMPOSED OF RX(1), RX(5), RX(10)
RX(26) A + J + S ==> T



A

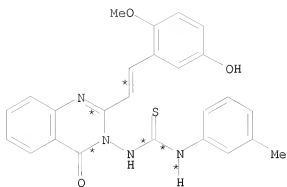


J



S

3
STEPS
→



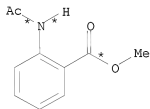
T
YIELD 30%

RX(1) RCT A 2719-08-6
RGT C 302-01-2 N2H4
PRO B 1898-06-2

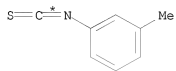
RX(5) RCT B 1898-06-2, J 621-30-7
PRO K 105886-56-4

RX(10) RCT K 105886-56-4, S 35431-26-6
PRO T 105886-61-1

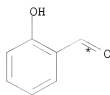
RX(27) OF 36 COMPOSED OF RX(1), RX(5), RX(11)
RX(27) A + J + N ==> U



A

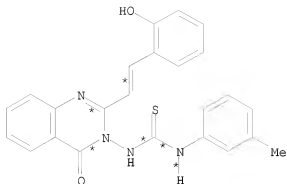


J



N

3
STEPS
→



U

YIELD 30%

RX(1) RCT A 2719-08-6
RGT C 302-01-2 N2H4
PRO B 1898-06-2

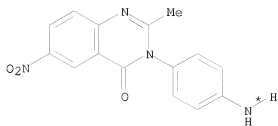
RX(5) RCT B 1898-06-2, J 621-30-7
PRO K 105886-56-4

RX(11) RCT K 105886-56-4, N 90-02-8
PRO U 105886-62-2

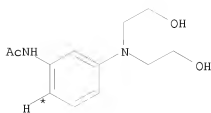
L3 ANSWER 189 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 105:228483 CASREACT
TITLE: Azo disperse dyes with 4-quinazolinone ring for dyeing polyester and nylon fibers
AUTHOR(S): Patel, M. H.; Patel, R. G.; Patel, V. S.
CORPORATE SOURCE: Dep. Chem., Sardar Patel Univ., Vallabh Vidyanagar, 388 120, India
SOURCE: Indian Journal of Textile Research (1986), 11(3), 164-7
CODEN: IJTRDU; ISSN: 0377-8436
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 6-Nitro-3-(p- or m-arylazophenyl)-2-methyl-4-quinazolinone dyes were prepared by coupling of diazotized 6-nitro-3-(aminophenyl)-2-methyl-4-quinazolinones and exhibited fair to good light fastness and good to excellent washing, rubbing, perspiration, and sublimation fastness on polyester and polyamide fibers. The dyes were characterized by elemental anal. and IR spectroscopy.

RX(29) OF 30 A + AS ==> AT

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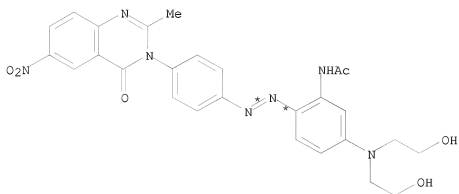


A



AS

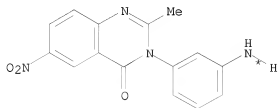
(29)



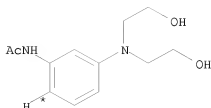
AT

RX(29) RCT A 105440-62-8, AS 92-02-4
PRO AT 105440-79-7

RX(30) OF 30 D + AS ==> AU

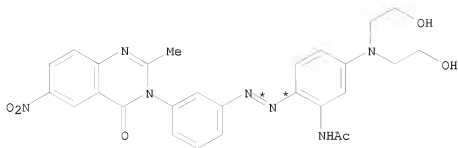


D



AS

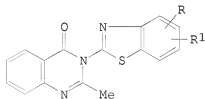
(30) 



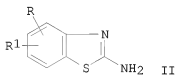
AU

RX(30) RCT D 105440-63-9, AS 92-02-4
PRO AU 105440-95-7

L3 ANSWER 190 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 105:226481 CASREACT
TITLE: Synthesis of some new
3-(2'-benzothiazolyl)-4(3H)-quinazolinones as
antifungal agents
AUTHOR(S): Lakhan, Ram; Rai, Babban J.
CORPORATE SOURCE: Dep. Chem., Banaras Hindu Univ., Varanasi, 221 005,
India
SOURCE: Journal of Chemical and Engineering Data (1986),
31(4), 501-2
CODEN: JCEAAX; ISSN: 0021-9568
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



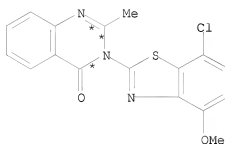
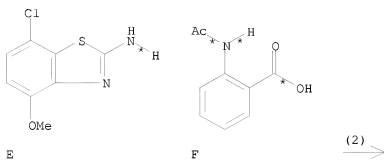
I



II

AB The title compds. I (R = 5-, 6-NO2, R1 = H; R = 4-MeO, R1 = 7-Cl; R = 4-NO2, R1 = 6-Cl, R = 4-Cl, R1 = 6-NO2) were prepared in 66-72% yield by the cyclization of o-MeCONHC6H4CO2H with aminobenzothiazoles II. I (R = 5-, 6-NO2, R1 = H; R = 4-Cl, R1 = 6-NO2) had fungicidal activity comparable with that of Dithan M-45.

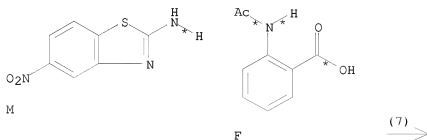
RX(2) OF 15 ...E + F ==> G



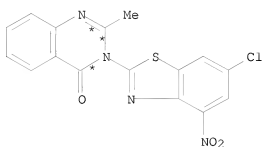
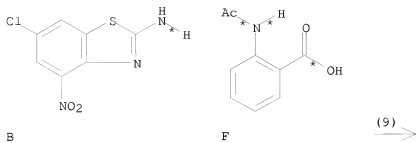
G

RX(2) RCT E 67618-12-6, F 89-52-1
 RGT H 7719-12-2 PC13
 PRO G 103852-54-6
 SOL 108-88-3 PhMe

RX(7) OF 15 ...M + F ==> Q



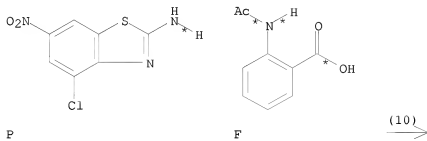
M

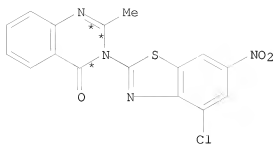


S

RX(9) RCT B 26488-55-1, F 89-52-1
 RGT H 7719-12-2 PC13
 PRO S 103852-55-7
 SOL 108-88-3 PhMe

RX(10) OF 15 ...P + F ==> T

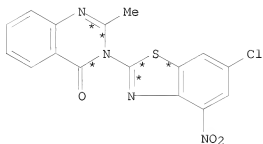
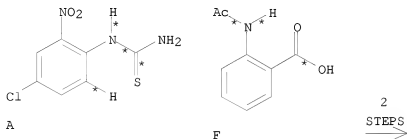




T

RX(10) RCT P 66188-30-5, F 89-52-1
 RGT H 7719-12-2 PC13
 PRO T 103852-56-8
 SOL 108-88-3 PhMe

RX(11) OF 15 COMPOSED OF RX(1), RX(9)
 RX(11) A + F ==> S



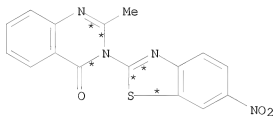
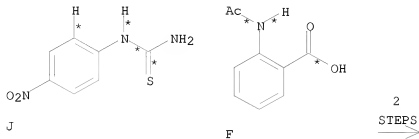
S

RX(1) RCT A 39535-50-7
 RGT C 7726-95-6 Br2
 PRO B 26488-55-1
 SOL 67-66-3 CHC13

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RX(9) RCT B 26488-55-1, F 89-52-1
 RGT H 7719-12-2 PC13
 PRO S 103852-55-7
 SOL 108-88-3 PhMe

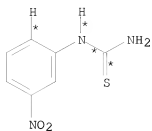
RX(12) OF 15 COMPOSED OF RX(3), RX(8)
 RX(12) J + F ==> R



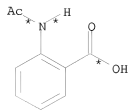
RX(3) RCT J 3696-22-8
 RGT C 7726-95-6 Br2
 PRO K 6285-57-0
 SOL 67-66-3 CHCl3

RX(8) RCT K 6285-57-0, F 89-52-1
 RGT H 7719-12-2 PC13
 PRO R 103852-53-5
 SOL 108-88-3 PhMe

RX(13) OF 15 COMPOSED OF RX(4), RX(7)
 RX(13) L + F ==> Q

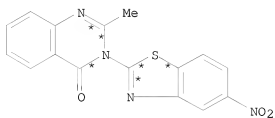


L



F

2
STEPS
→

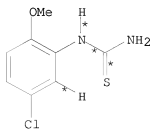


Q

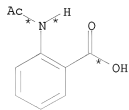
RX(4) RCT L 709-72-8
 RGT C 7726-95-6 Br2
 PRO M 73458-39-6
 SOL 67-66-3 CHCl3

RX(7) RCT M 73458-39-6, F 89-52-1
 RGT H 7719-12-2 PC13
 PRO Q 103852-52-4
 SOL 108-88-3 PhMe

RX(14) OF 15 COMPOSED OF RX(5), RX(2)
RX(14) N + F ==> G

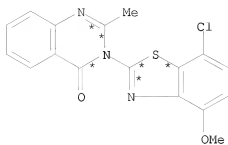


N



F

2
STEPS
→

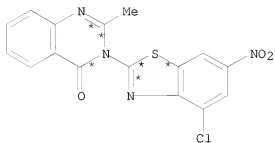
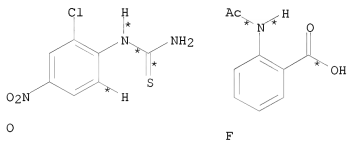


G

RX(5) RCT N 63980-69-8
 RGT C 7726-95-6 Br2
 PRO E 67618-12-6
 SOL 67-66-3 CHCl3

RX(2) RCT E 67618-12-6, F 89-52-1
 RGT H 7719-12-2 PC13
 PRO G 103852-54-6
 SOL 108-88-3 PhMe

RX(15) OF 15 COMPOSED OF RX(6), RX(10)
 RX(15) O + F ==> T

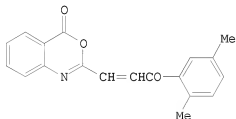


T

RX(6) RCT O 103852-57-9
 RGT C 7726-95-6 Br2
 PRO P 66188-30-5
 SOL 67-66-3 CHCl3

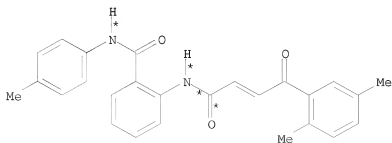
RX(10) RCT P 66188-30-5, F 89-52-1
 RGT H 7719-12-2 PC13
 PRO T 103852-56-8
 SOL 108-88-3 PhMe

L3 ANSWER 191 OF 258 CASREACT COPYRIGHT 2009 ACS on SIN
 ACCESSION NUMBER: 105:226465 CASREACT
 TITLE: Synthesis and some reactions of new
 3,1-benzoxazin-4-one derivatives
 AUTHOR(S): Soliman, E. A.; Attia, I. A.; Guber, A. M.
 CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
 SOURCE: Egyptian Journal of Chemistry (1985), 27(3), 297-308
 CODEN: EGJCA3; ISSN: 0367-0422
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



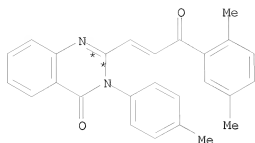
AB Benzoxazinone I was prepared by treating 2-HO2CC6H4NH2 with 2,5-Me2C6H3COCH:CHCOCl and cyclization of 2-HO2CC6H4NHCOCH:CHCOC6H3Me2-2,5 with Ac2O. I reacted with amines, hydrazines, NH2OH, ureas, and thioureas to form various heterocyclic derivs.

RX(4) OF 37 ...F ==> J



F

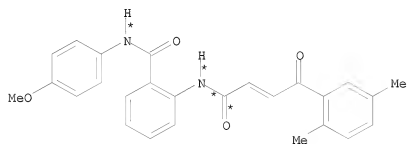
(4)
 →



J

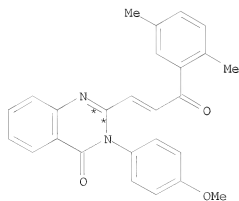
RX(4) RCT F 105493-09-2
 PRO J 105493-11-6
 CAT 108-24-7 Ac2O

RX(6) OF 37 ...I ==> M



I

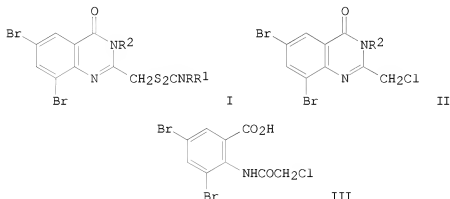
(6) →



M

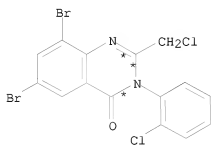
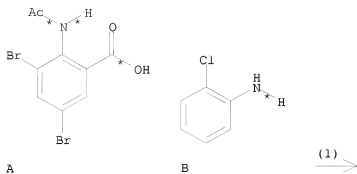
RX(6) RCT I 105493-10-5
 PRO M 105493-12-7
 CAT 108-24-7 Ac20

L3 ANSWER 192 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 105:133835 CASREACT
 TITLE: Synthesis and biological activities of
 [6,8-dibromo-3-aryl-3,4-dihydro-4-oxo-2-
 quinazolinyl]methyl N-substituted dithiocarbamates
 Rao, A. Devender; Shankar, C. Ravi; Reddy, V. Malla
 CORPORATE SOURCE: Coll. Pharm. Sci., Kakatiya Univ., Warangal, 506 009,
 India
 SOURCE: Current Science (1985), 54(15), 720-2
 CODEN: CUSCAM; ISSN: 0011-3891
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Quinazolinylmethyl dithiocarbamates I [R = H, cyclohexyl; R1 = Ph, C6H4Me-4, C6H4OEt-4, C6H4OMe-4, PhCH2, cyclohexyl, Me2N(CH2)3; RR1 = (CH2)4, (CH2)5, (CH2)2O(CH2)2, (CH2)2NPh(CH2)2] were prepared by condensation of (chloromethyl)quinazoline II (R2 = C6H4Cl-2, CH2C6H4OMe-2) with RR1NCS2H. A mixture of anthranilic acid III, 2-chloroaniline, and POCl3 in PhMe was refluxed at 130-140° for 3 h to give 72% II (R2 = C6H4Cl-2). I showed fungicidal and insecticidal activity.

RX(1) OF 40 A + B ==> C...

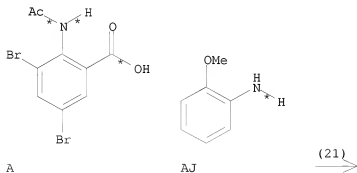


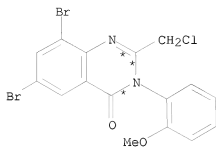
C

YIELD 72%

RX(1) RCT A 16610-45-0, B 95-51-2
 RGT D 10025-87-3 POC13
 PRO C 104308-98-7

RX(21) OF 40 A + AJ ==> AA...



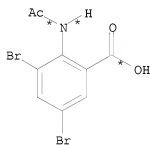


AA

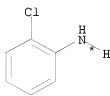
RX(21) RCT A 16610-45-0, AJ 90-04-0
 RGT D 10025-87-3 POC13
 PRO AA 104308-99-8

RX(22) OF 40 COMPOSED OF RX(1), RX(2)

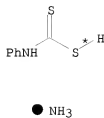
RX(22) A + B + E ==> F



A

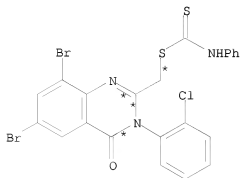


B



E

2
STEPS
→



F

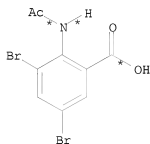
RX(1) RCT A 16610-45-0, B 95-51-2

10/ 562,112

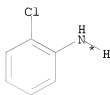
RGT D 10025-87-3 POC13
PRO C 104308-98-7

RX(2) RCT C 104308-98-7, E 1074-52-8
PRO F 104329-30-8

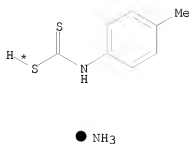
RX(23) OF 40 COMPOSED OF RX(1), RX(3)
RX(23) A + B + G ==> H



A

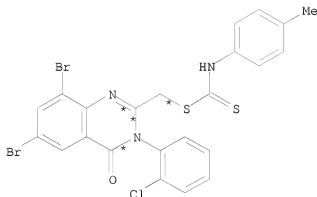


B



G

2
STEPS
→



H

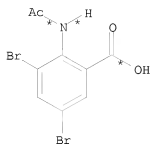
RX(1) RCT A 16610-45-0, B 95-51-2
RGT D 10025-87-3 POC13
PRO C 104308-98-7

RX(3) RCT C 104308-98-7, G 13036-91-4
PRO H 104308-78-3

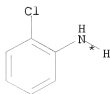
RX(24) OF 40 COMPOSED OF RX(1), RX(4)

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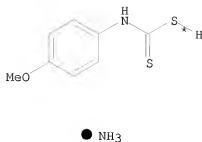
RX(24) A + B + I ==> J



A



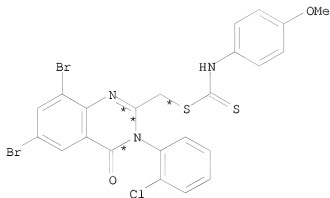
B



I

● NH₃

2
STEPS
→

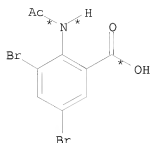


J

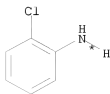
RX(1) RCT A 16610-45-0, B 95-51-2
RGT D 10025-87-3 POC13
PRO C 104308-98-7

RX(4) RCT C 104308-98-7, I 15866-98-5
PRO J 104308-79-4

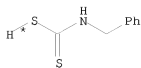
RX(25) OF 40 COMPOSED OF RX(1), RX(5)
RX(25) A + B + K ==> L



A



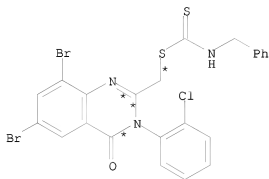
B



K



2
STEPS
→

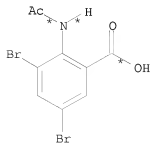


L

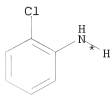
RX(1) RCT A 16610-45-0, B 95-51-2
RGT D 10025-87-3 POC13
PRO C 104308-98-7

RX(5) RCT C 104308-98-7, K 41270-27-3
PRO L 104308-80-7

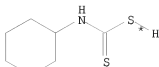
RX(26) OF 40 COMPOSED OF RX(1), RX(6)
RX(26) A + B + M ==> N



A



B

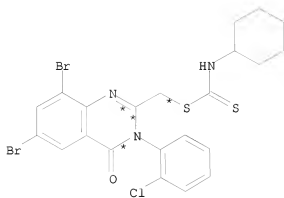


M



10/ 562,112

2
STEPS
→

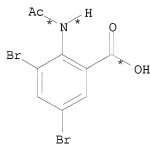


N

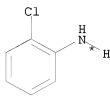
RX(1) RCT A 16610-45-0, B 95-51-2
RGT D 10025-87-3 POC13
PRO C 104308-98-7

RX(6) RCT C 104308-98-7, M 66917-87-1
PRO N 104329-32-0

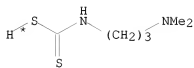
RX(27) OF 40 COMPOSED OF RX(1), RX(7)
RX(27) A + B + O ==> P



A



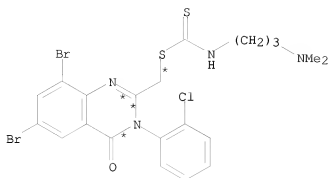
B



O

● NH₃

2
STEPS
→



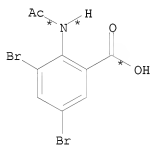
P

RX(1) RCT A 16610-45-0, B 95-51-2
 RGT D 10025-87-3 POC13
 PRO C 104308-98-7

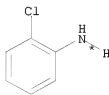
RX(7) RCT C 104308-98-7, O 200131-07-3
 PRO P 104308-81-8

RX(28) OF 40 COMPOSED OF RX(1), RX(8)

RX(28) A + B + Q ==> R



A

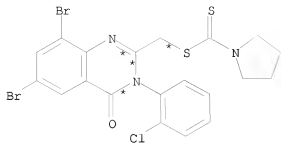


B

● NH₃

Q

2
 STEPS
 →

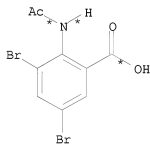


R
YIELD 72%

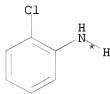
RX(1) RCT A 16610-45-0, B 95-51-2
RGT D 10025-87-3 POC13
PRO C 104308-98-7

RX(8) RCT C 104308-98-7, Q 5108-96-3
PRO R 104329-33-1

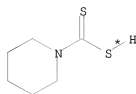
RX(29) OF 40 COMPOSED OF RX(1), RX(9)
RX(29) A + B + S ==> T



A

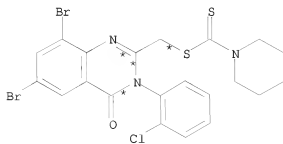


B



● NH₃
S

2
STEPS
→



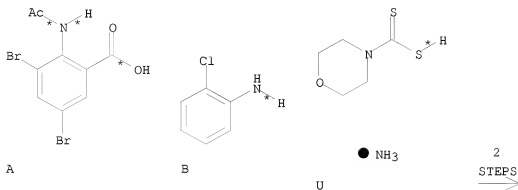
T

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RX(1) RCT A 16610-45-0, B 95-51-2
 RGT D 10025-87-3 POC13
 PRO C 104308-98-7

RX(9) RCT C 104308-98-7, S 49791-55-1
 PRO T 104308-82-9

RX(30) OF 40 COMPOSED OF RX(1), RX(10)
 RX(30) A + B + U ==> V

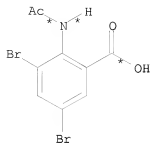


V

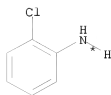
RX(1) RCT A 16610-45-0, B 95-51-2
 RGT D 10025-87-3 POC13
 PRO C 104308-98-7

RX(10) RCT C 104308-98-7, U 49791-54-0
 PRO V 104308-83-0

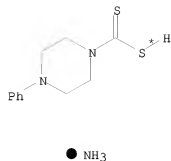
RX(31) OF 40 COMPOSED OF RX(1), RX(11)
 RX(31) A + B + W ==> X



A

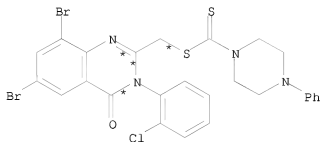


B



W

2
STEPS
→



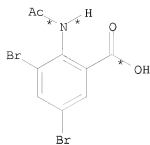
X

RX(1) RCT A 16610-45-0, B 95-51-2
RGT D 10025-87-3 POC13
PRO C 104308-98-7

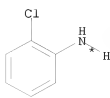
RX(11) RCT C 104308-98-7, W 100805-68-3
PRO X 104308-84-1

RX(32) OF 40 COMPOSED OF RX(1), RX(12)

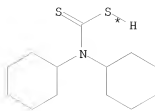
RX(32) A + B + Y ==> Z



A



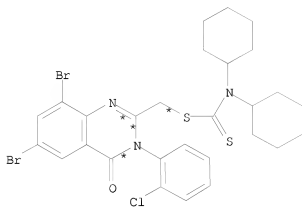
B



● NH₃

Y

2
STEPS
→

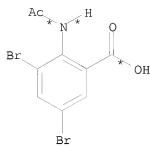


Z

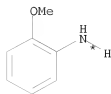
RX(1) RCT A 16610-45-0, B 95-51-2
 RGT D 10025-87-3 POC13
 PRO C 104308-98-7

RX(12) RCT C 104308-98-7, Y 100805-67-2
 PRO Z 104308-85-2

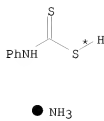
RX(33) OF 40 COMPOSED OF RX(21), RX(13)
RX(33) A + AJ + E ==> AB



A

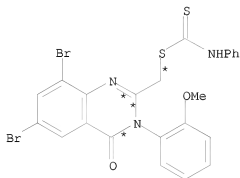


AJ



E

2
STEPS
→

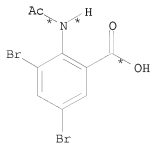


AB

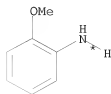
RX(21) RCT A 16610-45-0, AJ 90-04-0
RGT D 10025-87-3 POC13
PRO AA 104308-99-8

RX(13) RCT AA 104308-99-8, E 1074-52-8
PRO AB 104308-86-3

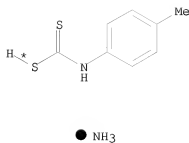
RX(34) OF 40 COMPOSED OF RX(21), RX(14)
RX(34) A + AJ + G ==> AC



A



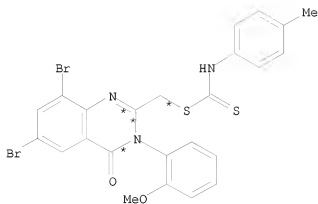
AJ



G

10/ 562,112

2
STEPS
→

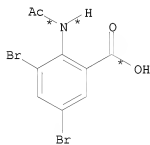


AC

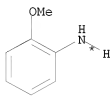
RX(21) RCT A 16610-45-0, AJ 90-04-0
RGT D 10025-87-3 POC13
PRO AA 104308-99-8

RX(14) RCT AA 104308-99-8, G 13036-91-4
PRO AC 104308-87-4

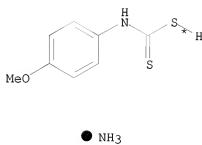
RX(35) OF 40 COMPOSED OF RX(21), RX(15)
RX(35) A + AJ + I ==> AD



A



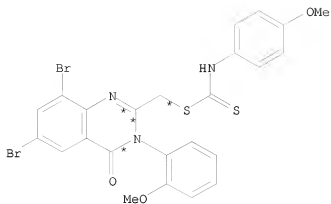
AJ



I

● NH₃

2
STEPS
→

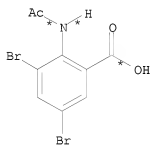


AD

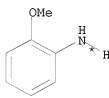
RX(21) RCT A 16610-45-0, AJ 90-04-0
 RGT D 10025-87-3 POC13
 PRO AA 104308-99-8

RX(15) RCT AA 104308-99-8, I 15866-98-5
 PRO AD 104308-89-6

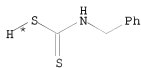
RX(36) OF 40 COMPOSED OF RX(21), RX(16)
 RX(36) A + AJ + K ==> AE



A



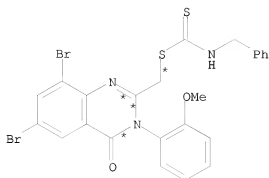
AJ



K



2
 STEPS
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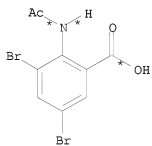


AE

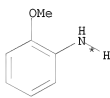
RX(21) RCT A 16610-45-0, AJ 90-04-0
 RGT D 10025-87-3 POC13
 PRO AA 104308-99-8

RX(16) RCT AA 104308-99-8, K 41270-27-3
 PRO AE 104308-90-9

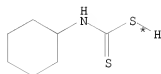
RX(37) OF 40 COMPOSED OF RX(21), RX(17)
 RX(37) A + AJ + M ==> AF



A



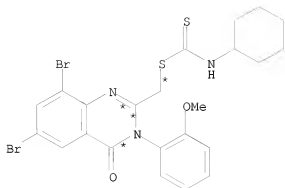
AJ



M

● NH₃

2
 STEPS
 →

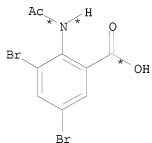


AF

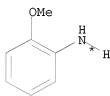
RX(21) RCT A 16610-45-0, AJ 90-04-0
 RGT D 10025-87-3 POC13
 PRO AA 104308-99-8

RX(17) RCT AA 104308-99-8, M 66917-87-1
 PRO AF 104308-91-0

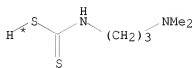
RX(38) OF 40 COMPOSED OF RX(21), RX(18)
 RX(38) A + AJ + O ==> AG



A



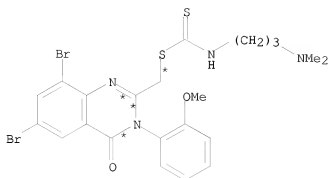
AJ



O



2
 STEPS
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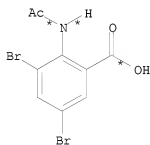


AG

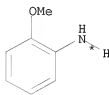
RX(21) RCT A 16610-45-0, AJ 90-04-0
 RGT D 10025-87-3 POC13
 PRO AA 104308-99-8

RX(18) RCT AA 104308-99-8, O 200131-07-3
 PRO AG 104308-92-1

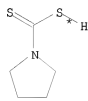
RX(39) OF 40 COMPOSED OF RX(21), RX(19)
 RX(39) A + AJ + Q ==> AH



A



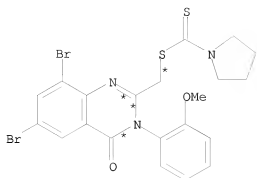
AJ



● NH3

Q

2
 STEPS
 ➔

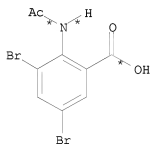


AH

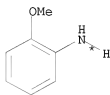
RX(21) RCT A 16610-45-0, AJ 90-04-0
RGT D 10025-87-3 POC13
PRO AA 104308-99-8

RX(19) RCT AA 104308-99-8, Q 5108-96-3
PRO AH 104308-93-2

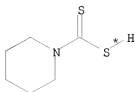
RX(40) OF 40 COMPOSED OF RX(21), RX(20)
RX(40) A + AJ + S ==> AI



A



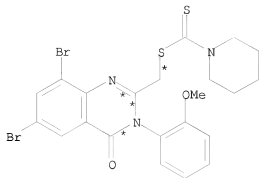
AJ



S

● NH₃

2
STEPS
→



AI

RX(21) RCT A 16610-45-0, AJ 90-04-0
 RGT D 10025-87-3 POC13
 PRO AA 104308-99-8

RX(20) RCT AA 104308-99-8, S 49791-55-1
 PRO AI 104308-94-3

L3 ANSWER 193 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:

105:97419 CASREACT

TITLE:

One pot synthesis of quinazoline derivatives by use of
 palladium catalyzed carbonylation
 Mori, Miwako; Kobayashi, Hiromi; Kimura, Masaya; Ban,
 Yoshio

AUTHOR(S):

CORPORATE SOURCE:

Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan

SOURCE:

Heterocycles (1985), 23(11), 2803-6

DOCUMENT TYPE:

Journal

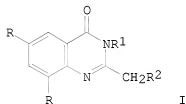
LANGUAGE:

English

GI

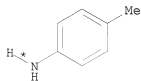
CAT 69058-45-3 Palladium, bis(acetato-κO)(triphenylphosphine)-
 SOL 680-31-9 HMPT

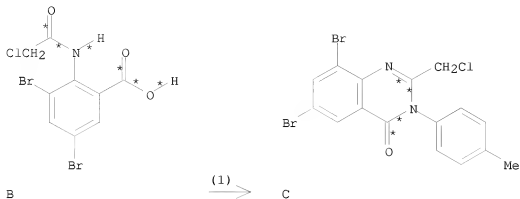
L3 ANSWER 194 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 105:97416 CASREACT
 TITLE: Synthesis and biological activities of certain
 derivatives of 3-aryl-4(3H)-quinazolinones. Part II
 AUTHOR(S): Rao, A. Devender; Shankar, C. Ravi; Reddy, P.
 Bhaghavan; Reddy, V. Malla
 CORPORATE SOURCE: Coll. Pharm. Sci., Kakatiya Univ., Warangal, 506 009,
 India
 SOURCE: Journal of the Indian Chemical Society (1985), 62(3),
 234-7
 CODEN: JICSAH; ISSN: 0019-4522
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB 3-Arylquinazolinones I [R = H, Br; R1 = 4-MeC6H4, 2-MeC6H4, 4-O2NC6H4, 2-O2NC6H4; R2 = NMe2, NEt2, N(CH2CH2OH)2, piperidino, morpholino, 4-AcNHC6H4SO2, etc.] were prepared from I (R2 = Cl), which were obtained by cyclocondensation of N-chloroacetylanthranilic acids with R1NH2 in the presence of PCl3. I are antifungal agents, I (R = H, R1 = 4-O2NC6H4, R2 = 4-AcNHC6H4SO2) giving total control of *Curvularia lunata* and *Fusarium oxysporum* at 800 µg/mL.

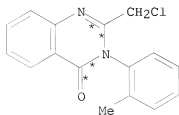
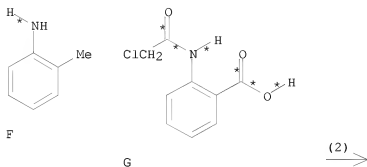
RX(1) OF 61 A + B ==> C...





RX(1) RCT A 106-49-0, B 103952-88-1
 RGT D 7719-12-2 PC13
 PRO C 103952-89-2
 SOL 108-88-3 PhMe

RX(2) OF 61 F + G \implies H...

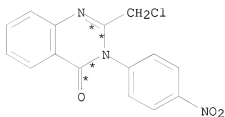
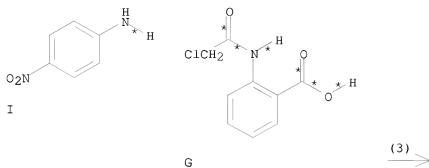


H

RX(2) RCT F 95-53-4, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO H 3166-54-9
 SOL 108-88-3 PhMe

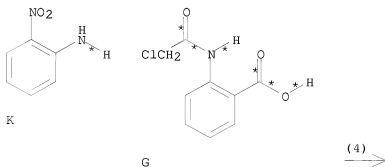
10/ 562,112

RX(3) OF 61 I + G ==> J...

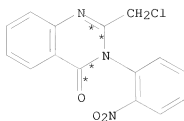


RX(3) RCT I 100-01-6, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO J 103952-90-5
 SOL 108-88-3 PhMe

RX(4) OF 61 K + G ==> L...



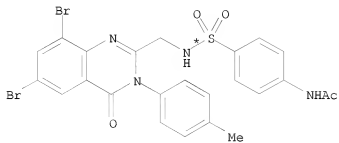
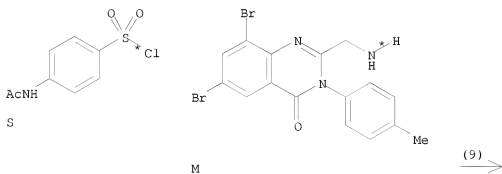
10/ 562,112



L

RX(4) RCT K 88-74-4, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO L 80096-22-6
 SOL 108-88-3 PhMe

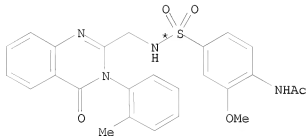
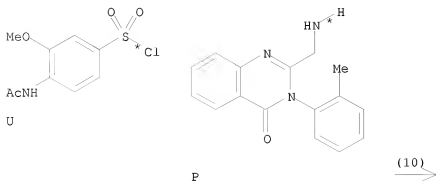
RX(9) OF 61 ...S + M ==> T



T

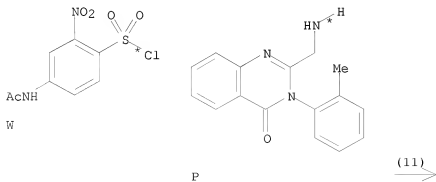
RX(9) RCT S 121-60-8, M 103952-91-6
 PRO T 103952-99-4
 SOL 110-86-1 Pyridine

RX(10) OF 61 ...U + P ==> V

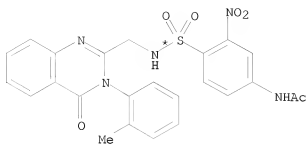


RX(10) RCT U 46713-94-4, P 80096-33-9
 PRO V 103953-04-4
 SOL 110-86-1 Pyridine

RX(11) OF 61 ...W + P ==> X



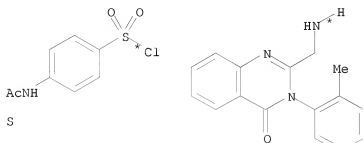
10/ 562,112



X

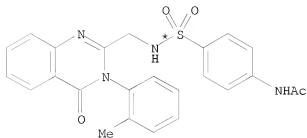
RX(11) RCT W 19300-50-6, P 80096-33-9
 PRO X 103953-05-5
 SOL 110-86-1 Pyridine

RX(12) OF 61 ...S + P ==> Y



P

(12) →

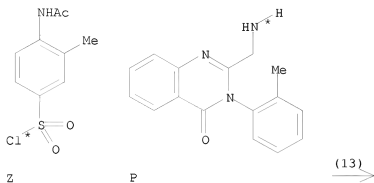


Y

RX(12) RCT S 121-60-8, P 80096-33-9
 PRO Y 103953-06-6
 SOL 110-86-1 Pyridine

10/ 562,112

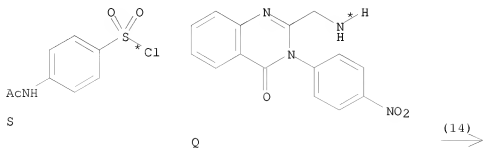
RX(13) OF 61 ...Z + P ==> AA



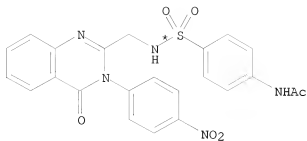
AA

RX(13) RCT Z 14988-21-7, P 80096-33-9
 PRO AA 103953-07-7
 SOL 110-86-1 Pyridine

RX(14) OF 61 ...S + Q ==> AB



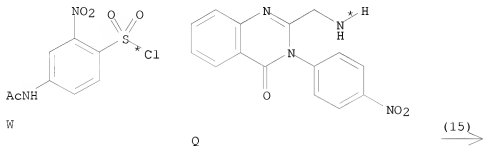
10/ 562,112



AB

RX(14) RCT S 121-60-8, Q 103952-92-7
 PRO AB 103953-00-0
 SOL 110-86-1 Pyridine

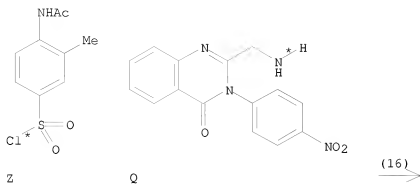
RX(15) OF 61 ...W + Q ==> AC



AC

RX(15) RCT W 19300-50-6, Q 103952-92-7
 PRO AC 103953-01-1
 SOL 110-86-1 Pyridine

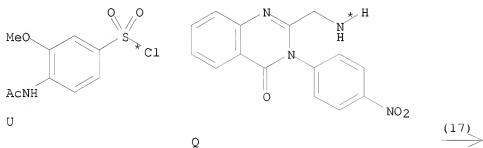
RX(16) OF 61 ...Z + Q ==> AD



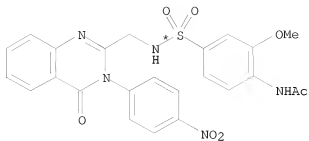
AD

RX(16) RCT Z 14988-21-7, Q 103952-92-7
 PRO AD 103953-02-2
 SOL 110-86-1 Pyridine

RX(17) OF 61 ...U + Q ==> AE



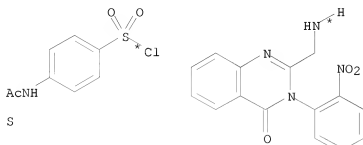
10/ 562,112



AE

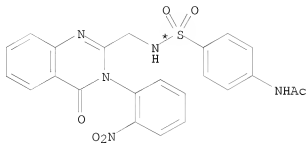
RX(17) RCT U 46713-94-4, Q 103952-92-7
 PRO AE 103953-03-3
 SOL 110-86-1 Pyridine

RX(18) OF 61 ...S + R ==> AF



R

(18)
 →

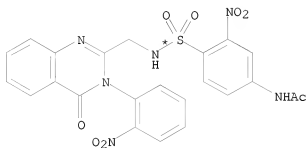
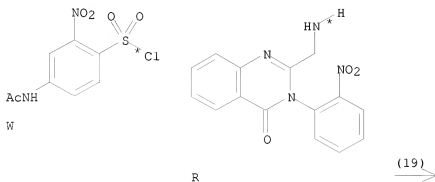


AF

RX(18) RCT S 121-60-8, R 103952-93-8
 PRO AF 103953-08-8
 SOL 110-86-1 Pyridine

10/ 562,112

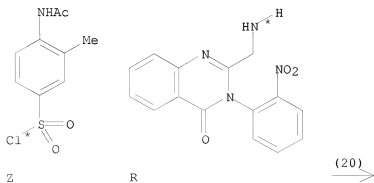
RX(19) OF 61 ...W + R ==> AG

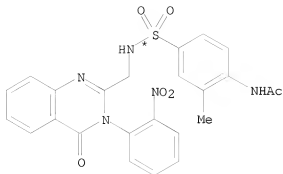


AG

RX(19) RCT W 19300-50-6, R 103952-93-8
 PRO AG 103953-09-9
 SOL 110-86-1 Pyridine

RX(20) OF 61 ...Z + R ==> AH

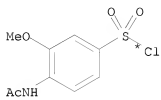




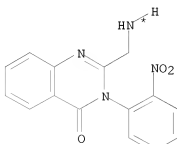
AH

RX(20) RCT Z 14988-21-7, R 103952-93-8
 PRO AH 103953-10-2
 SOL 110-86-1 Pyridine

RX(21) OF 61 ...U + R ==> AI

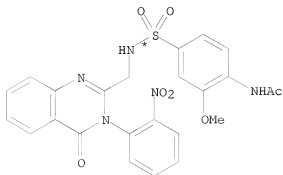


U



R

(21) →

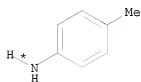


AI

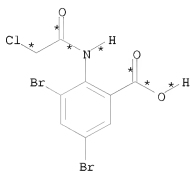
10/ 562,112

RX(21) RCT U 46713-94-4, R 103952-93-8
 PRO AI 103953-11-3
 SOL 110-86-1 Pyridine

RX(27) OF 61 COMPOSED OF RX(1), RX(5)
 RX(27) A + B ==> M

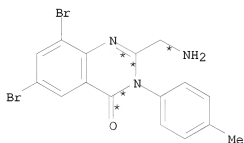


A



B

2
 STEPS
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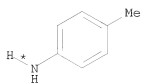
M

RX(1) RCT A 106-49-0, B 103952-88-1
 RGT D 7719-12-2 PC13
 PRO C 103952-89-2
 SOL 108-88-3 PhMe

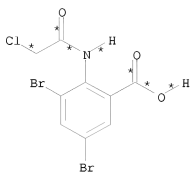
RX(5) RCT C 103952-89-2
 RGT N 7664-41-7 NH3
 PRO M 103952-91-6
 SOL 110-86-1 Pyridine

RX(28) OF 61 COMPOSED OF RX(1), RX(22)
 RX(28) A + B + AJ ==> AK

10/ 562,112



A

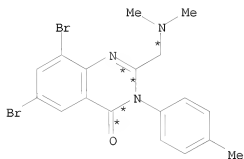


B



AJ

2
STEPS

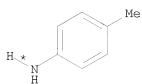


AK

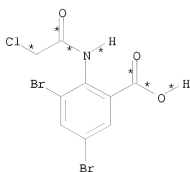
RX(1) RCT A 106-49-0, B 103952-88-1
RGT D 7719-12-2 PC13
PRO C 103952-89-2
SOL 108-88-3 PhMe

RX(22) RCT C 103952-89-2, AJ 124-40-3
PRO AK 103952-94-9
SOL 110-86-1 Pyridine

RX(29) OF 61 COMPOSED OF RX(1), RX(23)
RX(29) A + B + AL ==> AM



A

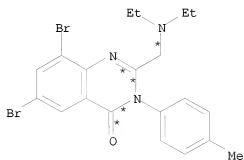


B



AL

2
STEPS
→

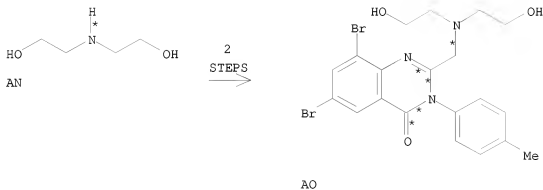
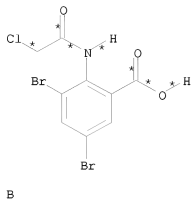
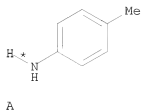


AM

RX(1) RCT A 106-49-0, B 103952-88-1
RGT D 7719-12-2 PC13
PRO C 103952-89-2
SOL 108-88-3 PhMe

RX(23) RCT C 103952-89-2, AL 109-89-7
PRO AM 103952-95-0
SOL 110-86-1 Pyridine

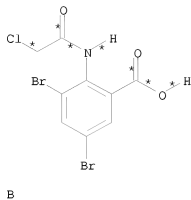
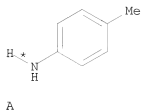
RX(30) OF 61 COMPOSED OF RX(1), RX(24)
RX(30) A + B + AN ==> AO



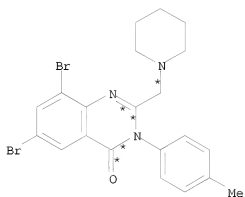
RX(1) RCT A 106-49-0, B 103952-88-1
 RGT D 7719-12-2 PC13
 PRO C 103952-89-2
 SOL 108-88-3 PhMe

RX(24) RCT C 103952-89-2, AN 111-42-2
 PRO AO 103952-96-1
 SOL 110-86-1 Pyridine

RX(31) OF 61 COMPOSED OF RX(1), RX(25)
 RX(31) A + B + AP ==> AQ



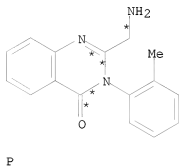
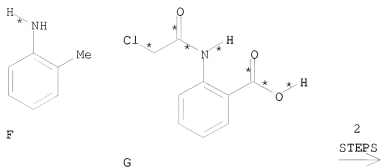
2
STEPS
→



RX(1) RCT A 106-49-0, B 103952-88-1
RGT D 7719-12-2 PC13
PRO C 103952-89-2
SOL 108-88-3 PhMe

RX(25) RCT C 103952-89-2, AP 110-89-4
PRO AQ 103952-97-2
SOL 110-86-1 Pyridine

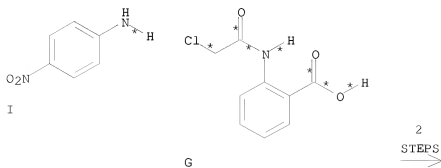
RX(33) OF 61 COMPOSED OF RX(2), RX(6)
RX(33) F + G ==> P

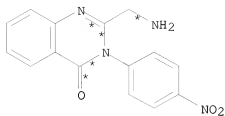


RX(2) RCT F 95-53-4, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO H 3166-54-9
 SOL 108-88-3 PhMe

RX(6) RCT H 3166-54-9
 RGT N 7664-41-7 NH3
 PRO P 80096-33-9
 SOL 110-86-1 Pyridine

RX(34) OF 61 COMPOSED OF RX(3), RX(7)
 RX(34) I + G ==> Q





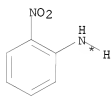
Q

RX(3) RCT I 100-01-6, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO J 103952-90-5
 SOL 108-88-3 PhMe

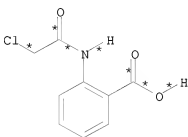
RX(7) RCT J 103952-90-5
 RGT N 7664-41-7 NH3
 PRO Q 103952-92-7
 SOL 110-86-1 Pyridine

RX(35) OF 61 COMPOSED OF RX(4), RX(8)

RX(35) K + G ==> R

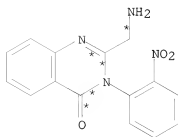


K



G

2
 STEPS
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R

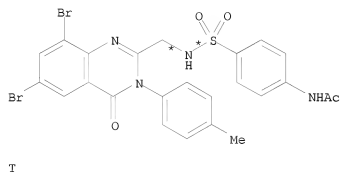
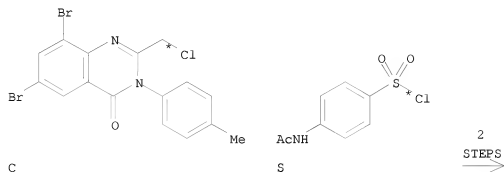
10/ 562,112

RX(4) RCT K 88-74-4, G 14422-49-2
RGT D 7719-12-2 PC13
PRO L 80096-22-6
SOL 108-88-3 PhMe

RX(8) RCT L 80096-22-6
RGT N 7664-41-7 NH3
PRO R 103952-93-8
SOL 110-86-1 Pyridine

RX(36) OF 61 COMPOSED OF RX(5), RX(9)

RX(36) C + S ==> T



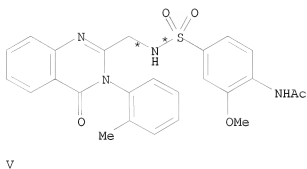
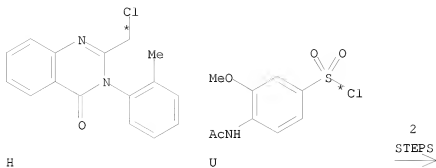
RX(5) RCT C 103952-89-2
RGT N 7664-41-7 NH3
PRO M 103952-91-6
SOL 110-86-1 Pyridine

RX(9) RCT S 121-60-8, M 103952-91-6
PRO T 103952-99-4
SOL 110-86-1 Pyridine

RX(37) OF 61 COMPOSED OF RX(6), RX(10)

RX(37) H + U ==> V

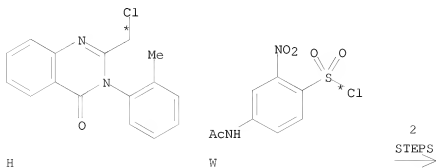
10/ 562,112

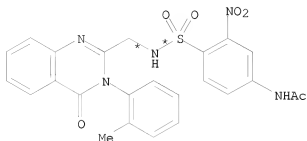


RX(6) RCT H 3166-54-9
RGT N 7664-41-7 NH3
PRO P 80096-33-9
SOL 110-86-1 Pyridine

RX(10) RCT U 46713-94-4, P 80096-33-9
PRO V 103953-04-4
SOL 110-86-1 Pyridine

RX(38) OF 61 COMPOSED OF RX(6), RX(11)
RX(38) H + W ==> X



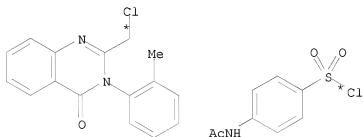


X

RX(6) RCT H 3166-54-9
 RGT N 7664-41-7 NH3
 PRO P 80096-33-9
 SOL 110-86-1 Pyridine

RX(11) RCT W 19300-50-6, P 80096-33-9
 PRO X 103953-05-5
 SOL 110-86-1 Pyridine

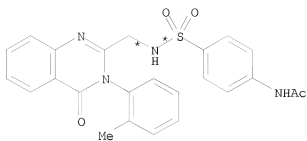
RX(39) OF 61 COMPOSED OF RX(6), RX(12)
 RX(39) H + S ==> Y



H

S

2
 STEPS
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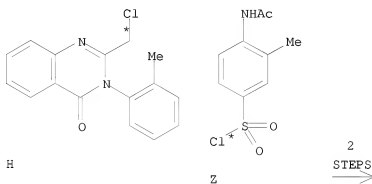


Y

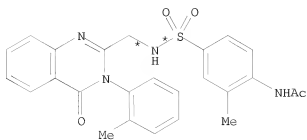
RX(6) RCT H 3166-54-9
 RGT N 7664-41-7 NH3
 PRO P 80096-33-9
 SOL 110-86-1 Pyridine

RX(12) RCT S 121-60-8, P 80096-33-9
 PRO Y 103953-06-6
 SOL 110-86-1 Pyridine

RX(40) OF 61 COMPOSED OF RX(6), RX(13)
 RX(40) H + Z ==> AA



AA

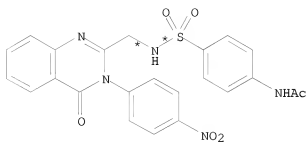
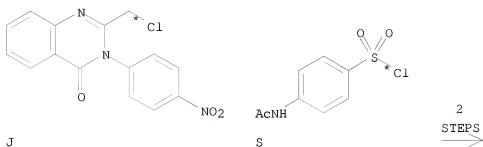


RX(6) RCT H 3166-54-9
 RGT N 7664-41-7 NH3
 PRO P 80096-33-9
 SOL 110-86-1 Pyridine

RX(13) RCT Z 14988-21-7, P 80096-33-9
 PRO AA 103953-07-7
 SOL 110-86-1 Pyridine

RX(41) OF 61 COMPOSED OF RX(7), RX(14)

RX(41) J + S ==> AB



AB

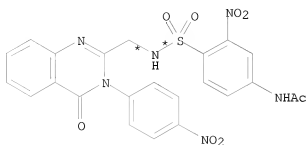
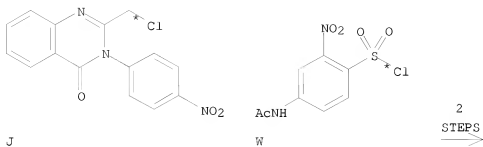
RX(7) RCT J 103952-90-5
 RGT N 7664-41-7 NH3
 PRO Q 103952-92-7
 SOL 110-86-1 Pyridine

RX(14) RCT S 121-60-8, Q 103952-92-7
 PRO AB 103953-00-0
 SOL 110-86-1 Pyridine

RX(42) OF 61 COMPOSED OF RX(7), RX(15)

RX(42) J + W ==> AC

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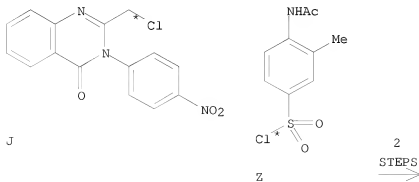


AC

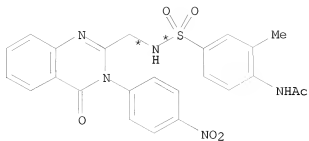
RX(7) RCT J 103952-90-5
 RGT N 7664-41-7 NH3
 PRO Q 103952-92-7
 SOL 110-86-1 Pyridine

RX(15) RCT W 19300-50-6, Q 103952-92-7
 PRO AC 103953-01-1
 SOL 110-86-1 Pyridine

RX(43) OF 61 COMPOSED OF RX(7), RX(16)
 RX(43) J + Z ==> AD



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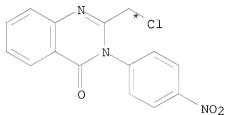


AD

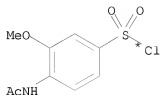
RX(7) RCT J 103952-90-5
 RGT N 7664-41-7 NH3
 PRO Q 103952-92-7
 SOL 110-86-1 Pyridine

RX(16) RCT Z 14988-21-7, Q 103952-92-7
 PRO AD 103953-02-2
 SOL 110-86-1 Pyridine

RX(44) OF 61 COMPOSED OF RX(7), RX(17)
 RX(44) J + U ==> AE

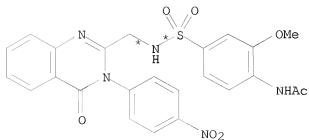


J



U

2
 STEPS
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AE

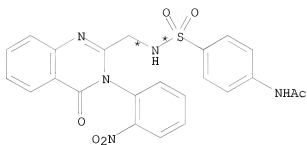
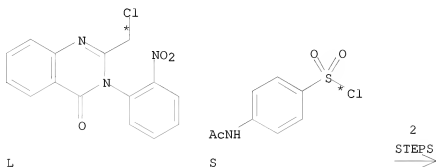
RX(7) RCT J 103952-90-5

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RGT N 7664-41-7 NH3
PRO Q 103952-92-7
SOL 110-86-1 Pyridine

RX(17) RCT U 46713-94-4, Q 103952-92-7
PRO AE 103953-03-3
SOL 110-86-1 Pyridine

RX(45) OF 61 COMPOSED OF RX(8), RX(18)
RX(45) L + S ==> AF

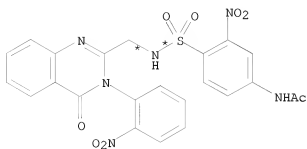
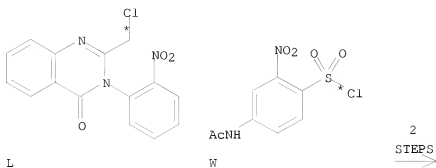


AF

RX(8) RCT L 80096-22-6
RGT N 7664-41-7 NH3
PRO R 103952-93-8
SOL 110-86-1 Pyridine

RX(18) RCT S 121-60-8, R 103952-93-8
PRO AF 103953-08-8
SOL 110-86-1 Pyridine

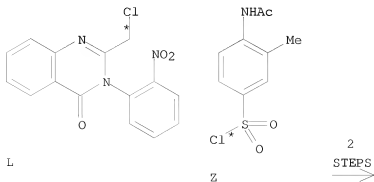
RX(46) OF 61 COMPOSED OF RX(8), RX(19)
RX(46) L + W ==> AG

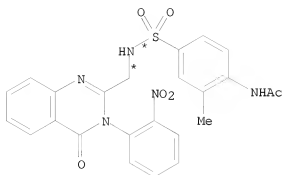


RX(8) RCT L 80096-22-6
 RGT N 7664-41-7 NH3
 PRO R 103952-93-8
 SOL 110-86-1 Pyridine

RX(19) RCT W 19300-50-6, R 103952-93-8
 PRO AG 103953-09-9
 SOL 110-86-1 Pyridine

RX(47) OF 61 COMPOSED OF RX(8), RX(20)
 RX(47) L + Z ==> AH





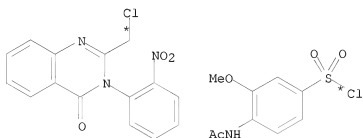
AH

RX(8) RCT L 80096-22-6
 RGT N 7664-41-7 NH3
 PRO R 103952-93-8
 SOL 110-86-1 Pyridine

RX(20) RCT Z 14988-21-7, R 103952-93-8
 PRO AH 103953-10-2
 SOL 110-86-1 Pyridine

RX(48) OF 61 COMPOSED OF RX(8), RX(21)

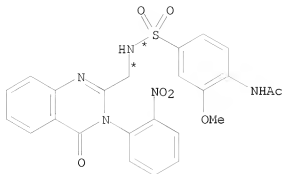
RX(48) L + U ==> AI



L

U

2
 STEPS
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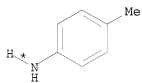


AI

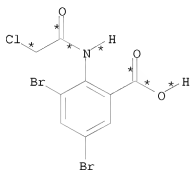
RX(8) RCT L 80096-22-6
 RGT N 7664-41-7 NH3
 PRO R 103952-93-8
 SOL 110-86-1 Pyridine

RX(21) RCT U 46713-94-4, R 103952-93-8
 PRO AI 103953-11-3
 SOL 110-86-1 Pyridine

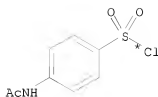
RX(49) OF 61 COMPOSED OF RX(1), RX(5), RX(9)
 RX(49) A + B + S ==> T



A

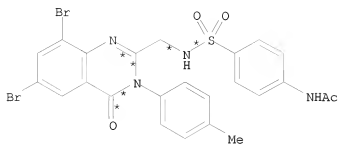


B



S

3
 STEPS
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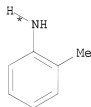
T

RX(1) RCT A 106-49-0, B 103952-88-1
 RGT D 7719-12-2 PC13
 PRO C 103952-89-2
 SOL 108-88-3 PhMe

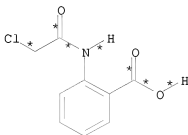
RX(5) RCT C 103952-89-2
 RGT N 7664-41-7 NH3
 PRO M 103952-91-6
 SOL 110-86-1 Pyridine

RX(9) RCT S 121-60-8, M 103952-91-6
 PRO T 103952-99-4
 SOL 110-86-1 Pyridine

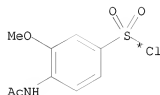
RX(50) OF 61 COMPOSED OF RX(2), RX(6), RX(10)
 RX(50) F + G + U ==> V



F



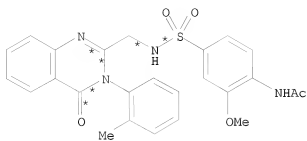
G



U

3
 STEPS
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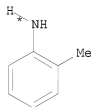
V

RX(2) RCT F 95-53-4, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO H 3166-54-9
 SOL 108-88-3 PhMe

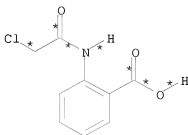
RX(6) RCT H 3166-54-9
 RGT N 7664-41-7 NH3
 PRO P 80096-33-9
 SOL 110-86-1 Pyridine

RX(10) RCT U 46713-94-4, P 80096-33-9
 PRO V 103953-04-4
 SOL 110-86-1 Pyridine

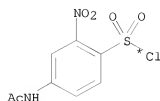
RX(51) OF 61 COMPOSED OF RX(2), RX(6), RX(11)
 RX(51) F + G + W ==> X



F

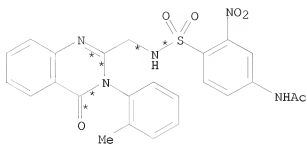


G



W

3
 STEPS
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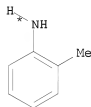
X

RX(2) RCT F 95-53-4, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO H 3166-54-9
 SOL 108-88-3 PhMe

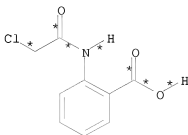
RX(6) RCT H 3166-54-9
 RGT N 7664-41-7 NH3
 PRO P 80096-33-9
 SOL 110-86-1 Pyridine

RX(11) RCT W 19300-50-6, P 80096-33-9
 PRO X 103953-05-5
 SOL 110-86-1 Pyridine

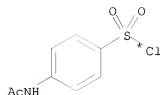
RX(52) OF 61 COMPOSED OF RX(2), RX(6), RX(12)
 RX(52) F + G + S ==> Y



F

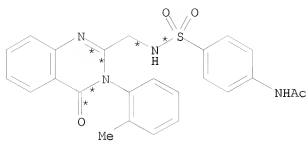


G



S

3
 STEPS
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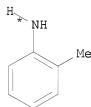
Y

RX(2) RCT F 95-53-4, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO H 3166-54-9
 SOL 108-88-3 PhMe

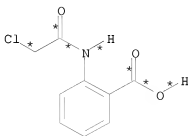
RX(6) RCT H 3166-54-9
 RGT N 7664-41-7 NH3
 PRO P 80096-33-9
 SOL 110-86-1 Pyridine

RX(12) RCT S 121-60-8, P 80096-33-9
 PRO Y 103953-06-6
 SOL 110-86-1 Pyridine

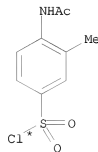
RX(53) OF 61 COMPOSED OF RX(2), RX(6), RX(13)
 RX(53) F + G + Z ==> AA



F

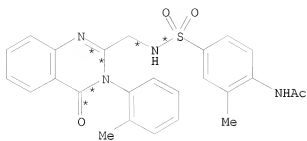


G



Z

3
 STEPS
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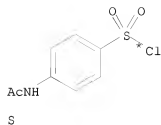
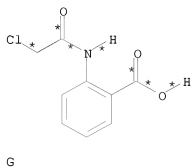
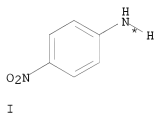
AA

RX(2) RCT F 95-53-4, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO H 3166-54-9
 SOL 108-88-3 PhMe

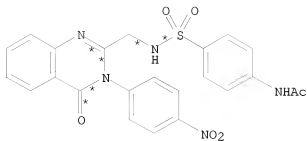
RX(6) RCT H 3166-54-9
 RGT N 7664-41-7 NH3
 PRO P 80096-33-9
 SOL 110-86-1 Pyridine

RX(13) RCT Z 14988-21-7, P 80096-33-9
 PRO AA 103953-07-7
 SOL 110-86-1 Pyridine

RX(54) OF 61 COMPOSED OF RX(3), RX(7), RX(14)
 RX(54) I + G + S ==> AB



3
 STEPS
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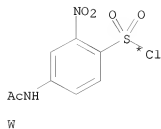
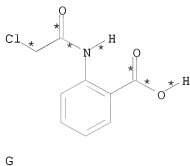
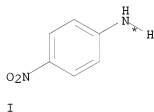
AB

RX(3) RCT I 100-01-6, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO J 103952-90-5
 SOL 108-88-3 PhMe

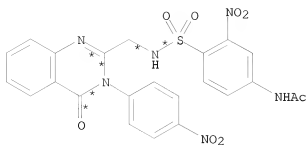
RX(7) RCT J 103952-90-5
 RGT N 7664-41-7 NH3
 PRO Q 103952-92-7
 SOL 110-86-1 Pyridine

RX(14) RCT S 121-60-8, Q 103952-92-7
 PRO AB 103953-00-0
 SOL 110-86-1 Pyridine

RX(55) OF 61 COMPOSED OF RX(3), RX(7), RX(15)
 RX(55) I + G + W ==> AC



3
 STEPS
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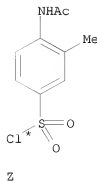
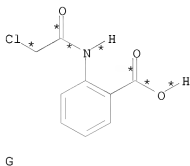
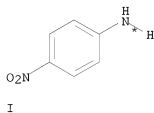
AC

RX(3) RCT I 100-01-6, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO J 103952-90-5
 SOL 108-88-3 PhMe

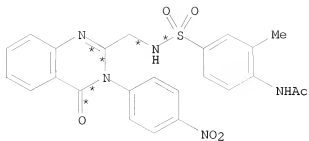
RX(7) RCT J 103952-90-5
 RGT N 7664-41-7 NH3
 PRO Q 103952-92-7
 SOL 110-86-1 Pyridine

RX(15) RCT W 19300-50-6, Q 103952-92-7
 PRO AC 103953-01-1
 SOL 110-86-1 Pyridine

RX(56) OF 61 COMPOSED OF RX(3), RX(7), RX(16)
 RX(56) I + G + Z ==> AD



3
 STEPS
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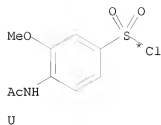
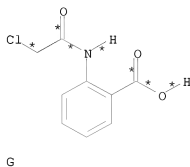
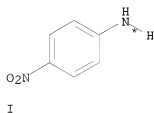
AD

RX(3) RCT I 100-01-6, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO J 103952-90-5
 SOL 108-88-3 PhMe

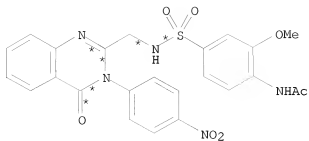
RX(7) RCT J 103952-90-5
 RGT N 7664-41-7 NH3
 PRO Q 103952-92-7
 SOL 110-86-1 Pyridine

RX(16) RCT Z 14988-21-7, Q 103952-92-7
 PRO AD 103953-02-2
 SOL 110-86-1 Pyridine

RX(57) OF 61 COMPOSED OF RX(3), RX(7), RX(17)
 RX(57) I + G + U ==> AE



3
 STEPS
 →



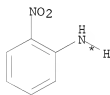
AE

RX(3) RCT I 100-01-6, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO J 103952-90-5
 SOL 108-88-3 PhMe

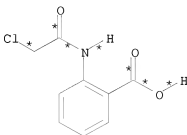
RX(7) RCT J 103952-90-5
 RGT N 7664-41-7 NH3
 PRO Q 103952-92-7
 SOL 110-86-1 Pyridine

RX(17) RCT U 46713-94-4, Q 103952-92-7
 PRO AE 103953-03-3
 SOL 110-86-1 Pyridine

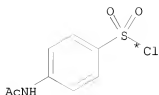
RX(58) OF 61 COMPOSED OF RX(4), RX(8), RX(18)
 RX(58) K + G + S ==> AF



K



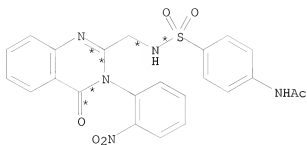
G



S

3
 STEPS
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10/ 562,112



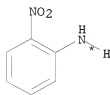
AF

RX(4) RCT K 88-74-4, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO L 80096-22-6
 SOL 108-88-3 PhMe

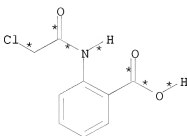
RX(8) RCT L 80096-22-6
 RGT N 7664-41-7 NH3
 PRO R 103952-93-8
 SOL 110-86-1 Pyridine

RX(18) RCT S 121-60-8, R 103952-93-8
 PRO AF 103953-08-8
 SOL 110-86-1 Pyridine

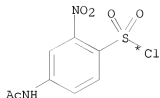
RX(59) OF 61 COMPOSED OF RX(4), RX(8), RX(19)
 RX(59) K + G + W ==> AG



K

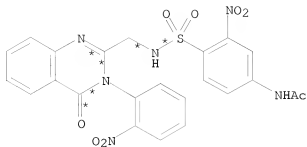


G



W

3
 STEPS
 ==>



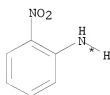
AG

RX(4) RCT K 88-74-4, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO L 80096-22-6
 SOL 108-88-3 PhMe

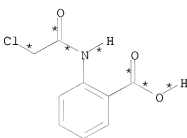
RX(8) RCT L 80096-22-6
 RGT N 7664-41-7 NH3
 PRO R 103952-93-8
 SOL 110-86-1 Pyridine

RX(19) RCT W 19300-50-6, R 103952-93-8
 PRO AG 103953-09-9
 SOL 110-86-1 Pyridine

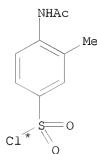
RX(60) OF 61 COMPOSED OF RX(4), RX(8), RX(20)
 RX(60) K + G + Z ==> AH



K

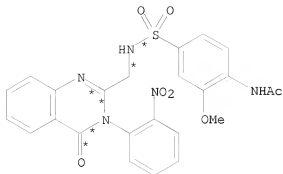


G



Z

3
 STEPS
 →



AI

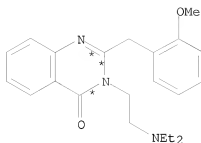
RX(4) RCT K 88-74-4, G 14422-49-2
 RGT D 7719-12-2 PC13
 PRO L 80096-22-6
 SOL 108-88-3 PhMe

RX(8) RCT L 80096-22-6
 RGT N 7664-41-7 NH3
 PRO R 103952-93-8
 SOL 110-86-1 Pyridine

RX(21) RCT U 46713-94-4, R 103952-93-8
 PRO AI 103953-11-3
 SOL 110-86-1 Pyridine

L3 ANSWER 195 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 105:60629 CASREACT
 TITLE: 2-Phenylalkyl-3-aminoalkyl-4(3H)-quinazolinones,
 pharmaceutical compositions and use
 INVENTOR(S): Sekiya, Tetsuo; Tsutsui, Mikio; Horii, Daijiro;
 Ishibashi, Akira
 PATENT ASSIGNEE(S): Mitsubishi Yuka Pharmaceutical Co., Ltd., Japan
 SOURCE: Eur. Pat. Appl., 58 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

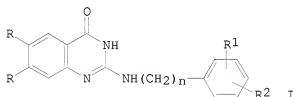
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 169537	A2	19860129	EP 1985-109193	19850723
EP 169537	A3	19870325		
EP 169537	B1	19900103		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
JP 61036273	A	19860220	JP 1984-154086	19840726
US 4668682	A	19870526	US 1985-753708	19850710
CA 1266266	A1	19900227	CA 1985-486793	19850715
AT 49199	T	19900115	AT 1985-109193	19850723



F

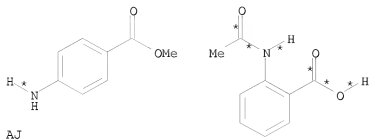
RX(3) RCT C 75256-36-9, E 100-36-7
PRO F 103316-51-4

L3 ANSWER 196 OF 258 CASREACT COPYRIGHT 2009 ACS on SIN
ACCESSION NUMBER: 104:186373 CASREACT
TITLE: Design and synthesis of
2-(arylamino)-4(3H)-quinazolinones as novel inhibitors
of rat lens aldose reductase
AUTHOR(S): DeRuiter, Jack; Brubaker, Abram N.; Millen, Jane;
Riley, Thomas N.
CORPORATE SOURCE: Sch. Pharm., Auburn Univ., Auburn, AL, 36849, USA
SOURCE: Journal of Medicinal Chemistry (1986), 29(5), 627-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



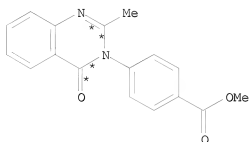
AB Title quinazolinones I (R = H, MeO; R1 = H, 4-HO, 4-CO2H, 4-SO3Na, R2 = H; R1 = 3-HO, R2 = CO2H; n = 0, 1) which possess several of the pharmacophore moieties necessary for binding to the inhibitor site of aldose reductase, were prepared and tested for their ability to inhibit crude aldose reductase obtained from rat lens. Only those quinazolinones that possess an acidic moiety on the (arylamino) substituent were found to display significant inhibitory activity. The most potent compound is I (R = MeO, R1 = 4-CO2H, R2 = H, n = 0) with an IC50 of 34 μ M, while the least potent is I (R = H, R1 = 4-HO, R2 = H, n = 0) with an IC50 of 75 μ M.

RX(16) OF 49 AJ + AK ==> AL...



AK

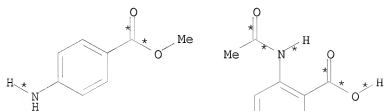
(16) \longrightarrow



AL

RX(16) RCT AJ 619-45-4, AK 89-52-1
 RGT AM 7719-12-2 PC13
 PRO AL 35218-84-9
 SOL 108-88-3 PhMe

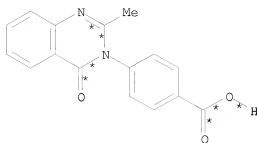
RX(31) OF 49 COMPOSED OF RX(16), RX(17)
 RX(31) AJ + AK \implies AO



AJ

AK

2
 STEPS \longrightarrow



AO

RX(16) RCT AJ 619-45-4, AK 89-52-1
 RGT AM 7719-12-2 PC13
 PRO AL 35218-84-9
 SOL 108-88-3 PhMe

RX(17) RCT AL 35218-84-9
 RGT X 7647-01-0 HCl
 PRO AO 4005-05-4
 SOL 7732-18-5 Water

L3 ANSWER 197 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 104:109677 CASREACT

TITLE: Quinazolinones

INVENTOR(S): Inoe, Kazumi; Oine, Toyao; Yamada, Yoshihisa; Ishida, Ryuichi; Ochiai, Takashi

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

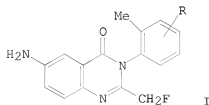
Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

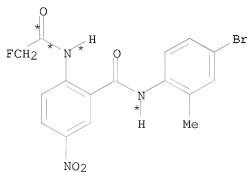
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60178817	A	19850912	JP 1984-33251	19840222
PRIORITY APPLN. INFO.:			JP 1984-33251	19840222

GI



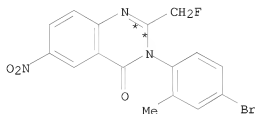
AB The title compds. (I; R = alkyl, alkoxy, halo), useful as muscle relaxants (no data), were prepared. Thus, a mixture of 4.16 g 5-nitroisatoic anhydride, 3.6 g 2,4-Me₂C₆H₃NH₂, and 25 mL xylene was refluxed for 30 min to give 82% 2,5-H₂N(O₂N)C₆H₃CONHC₆H₃Me₂-2,4, which (4.0 g) in THF containing pyridine was treated with 2.18 g FCH₂COCl at room temperature for 5 h to give 4.3 g 2,5-FCH₂CONH(O₂N)C₆H₃CONHC₆H₃Me₂-2,4, which (4.0 g) was heated with BF₃·Et₂O in HOAc at 100-105° for 30 min to give 2.6 g 2-(fluoromethyl)-3-(2,4-dimethylphenyl)-4-nitro-4(3H)-quinazolinone, reduction of which (2.0 g) with SnCl₂ gave 1.2 g I (R = 4-Me).

RX(2) OF 12 ...B ==> C...



B

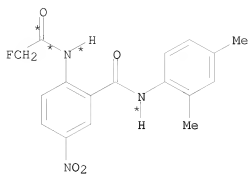
(2) →



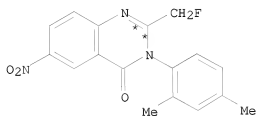
C

RX(2) RCT B 73832-54-9
PRO C 73832-62-9

RX(5) OF 12 ...F ==> G...



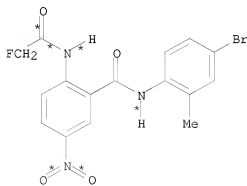
F

(5)
→

G

RX(5) RCT F 93670-44-1
 PRO G 93670-45-2

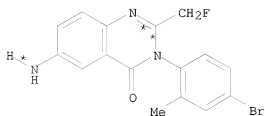
RX(8) OF 12 COMPOSED OF RX(2), RX(3)
 RX(8) B ==> D



B

2
STEPS
→

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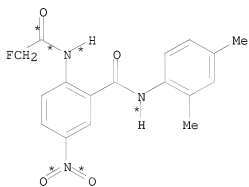
D

RX(2) RCT B 73832-54-9
PRO C 73832-62-9

RX(3) RCT C 73832-62-9
PRO D 73832-11-8

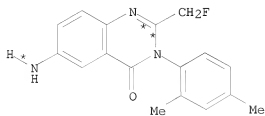
RX(10) OF 12 COMPOSED OF RX(5), RX(6)

RX(10) F ==> H



F

2
STEPS
→



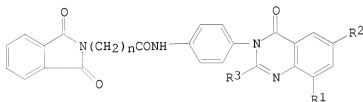
H

RX(5) RCT F 93670-44-1
PRO G 93670-45-2

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RX(6) RCT G 93670-45-2
PRO H 93670-47-4

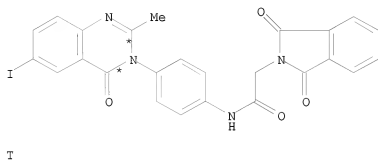
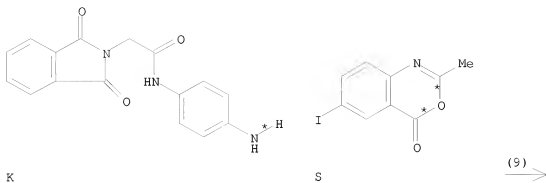
L3 ANSWER 198 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 104:81557 CASREACT
TITLE: Synthesis of 6,8-disubstituted
2-methyl/phenyl-3-[4-(3-phthalimido
acetamido/propionamido)]phenylquinazolin-4-ones as
anthelmintic agents
AUTHOR(S): Shukla, J. S.; Srivastava, Beena
CORPORATE SOURCE: Dep. Chem., Lucknow Univ., Lucknow, 226 001, India
SOURCE: Current Science (1985), 54(22), 1162-4
CODEN: CUSCAM; ISSN: 0011-3891
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

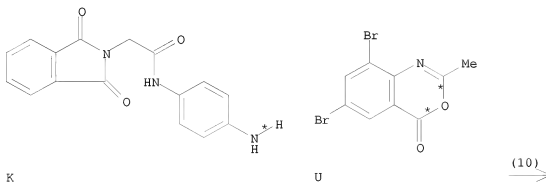
AB Twelve title compds. (I; R1 = H or Br; R2 = H, Br, or I; R3 = Me or Ph; and n = 1 or 2) were prepared, by reaction of 2-(p-aminophenylacetamido)phthalamide [100278-18-0] or its propionamido homolog [100278-21-5] with 6,8-disubstituted 2-phenylbenzoxazin-4-ones, and screened for anthelmintic activity in mice, rats, and hamsters. All I were inactive as cestodicidal agents. I(R1 = R2 = Br and R3 = Ph) [100278-22-6] was the most active agent against N. brasiliensis infestation in rats; I(R1 = R2 = H and R3 = Me) [100278-15-7] was most active against A. ceylanicum infestation in hamsters. Some structure-activity relations are discussed briefly.

RX(9) OF 39 K + S ==> T

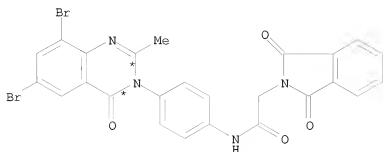


RX(9) RCT K 100278-18-0, S 40889-40-5
 PRO T 100278-10-2
 CAT 110-86-1 Pyridine

RX(10) OF 39 K + U ==> V



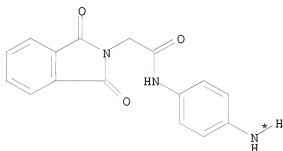
10/ 562,112



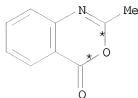
V

RX(10) RCT K 100278-18-0, U 40889-42-7
 PRO V 100278-11-3
 CAT 110-86-1 Pyridine

RX(11) OF 39 K + W ==> X

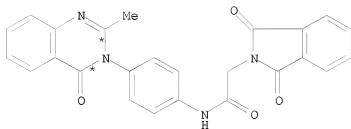


K



W

(11) →

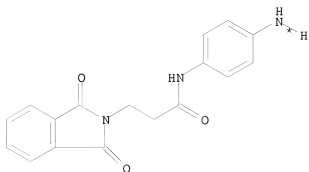


X

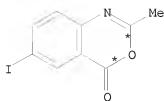
RX(11) RCT K 100278-18-0, W 525-76-8
 PRO X 100278-12-4
 CAT 110-86-1 Pyridine

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RX(15) OF 39 ...I + S ==> AB

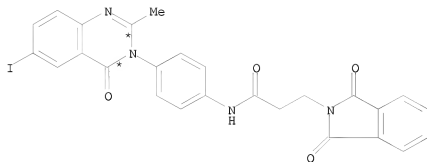


I



S

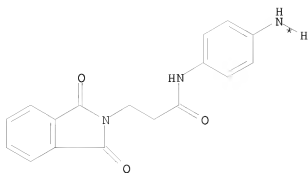
(15)
→



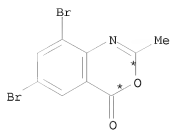
AB

RX(15) RCT I 100278-21-5, S 40889-40-5
PRO AB 100828-89-5
CAT 110-86-1 Pyridine

RX(16) OF 39 ...I + U ==> AC

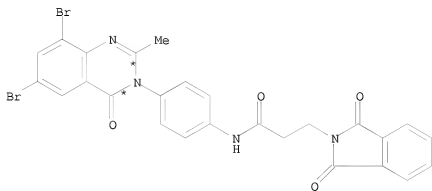


I



U

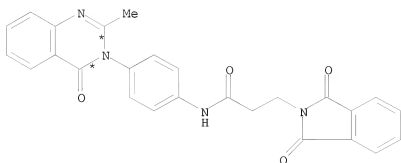
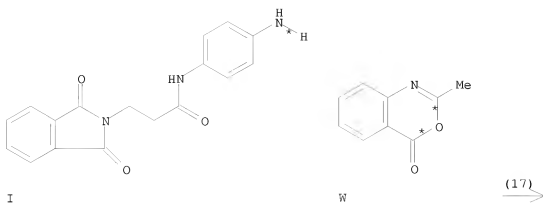
(16)



AC

RX(16) RCT I 100278-21-5, U 40889-42-7
 PRO AC 100278-16-8
 CAT 110-86-1 Pyridine

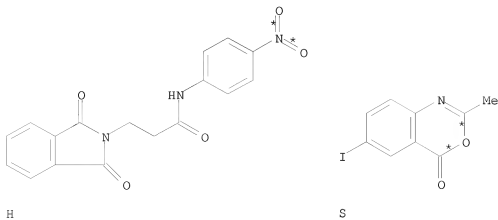
RX(17) OF 39 ...I + W ==> AD



AD

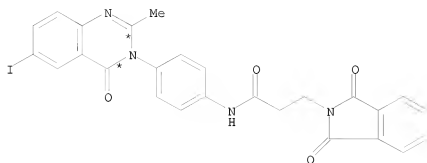
RX(17) RCT I 100278-21-5, W 525-76-8
 PRO AD 100278-15-7
 CAT 110-86-1 Pyridine

RX(24) OF 39 COMPOSED OF RX(5), RX(15)
 RX(24) H + S ==> AB



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2
STEPS
→

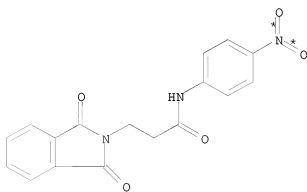


AB

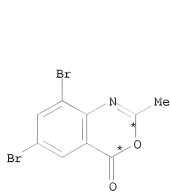
RX(5) RCT H 100278-17-9
RGT J 302-01-2 N2H4
PRO I 100278-21-5

RX(15) RCT I 100278-21-5, S 40889-40-5
PRO AB 100828-89-5
CAT 110-86-1 Pyridine

RX(25) OF 39 COMPOSED OF RX(5), RX(16)
RX(25) H + U ==> AC

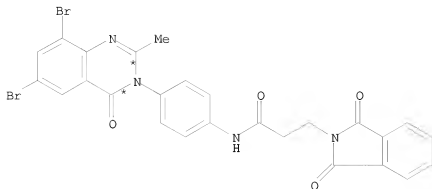


H



U

2
STEPS
→

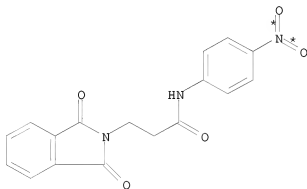


AC

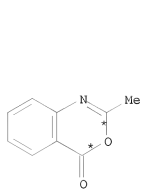
RX(5) RCT H 100278-17-9
RGT J 302-01-2 N2H4
PRO I 100278-21-5

RX(16) RCT I 100278-21-5, U 40889-42-7
PRO AC 100278-16-8
CAT 110-86-1 Pyridine

RX(26) OF 39 COMPOSED OF RX(5), RX(17)
RX(26) H + W ==> AD

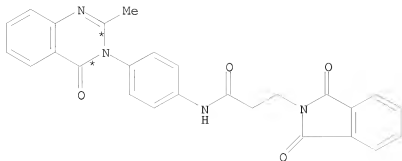


H



W

2
STEPS
→

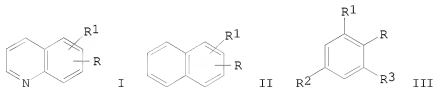


AD

RX(5) RCT H 100278-17-9
 RGT J 302-01-2 N2H4
 PRO I 100278-21-5

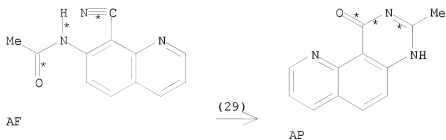
RX(17) RCT I 100278-21-5, W 525-76-8
 PRO AD 100278-15-7
 CAT 110-86-1 Pyridine

L3 ANSWER 199 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 103:104667 CASREACT
 TITLE: Studies on aromatic nitro compounds. V. A simple one-pot preparation of o-aminoaroylnitriles from some aromatic nitro compounds
 AUTHOR(S): Tomioka, Yukihiro; Ohkubo, Kimiko; Yamazaki, Motoyoshi
 CORPORATE SOURCE: Fac. Pharm. Sci., Fukuoka Univ., Fukuoka, 814-01, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(4), 1360-6
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



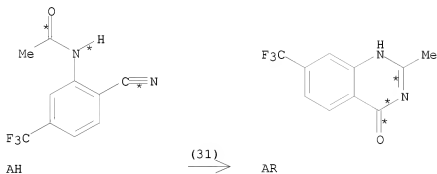
AB The reactions of aromatic nitro compds. I, II (R = H, R1 = NO2), and III (R, R1 = same, R2 = CF3, MeCO, PhCO, R3 = H ; R2 = R3 = CF3) with Et cyanoacetate and KOH in DMF followed by hydrolysis of the reaction mixture with HCl or NaOH gave the corresponding o-aminoaroylnitriles I-III (R = CN, R1 = NH2). Acetylation-cyclization reactions of the products were carried out.

RX(29) OF 55 ...AF ==> AP



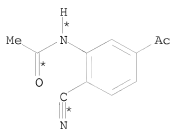
RX(29) RCT AF 98012-90-9
 RGT E 7647-01-0 HCl
 PRO AP 98012-97-6
 SOL 64-17-5 EtOH

RX(31) OF 55 ...AH ==> AR

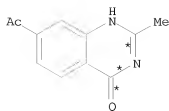


RX(31) RCT AH 98012-92-1
 RGT E 7647-01-0 HCl
 PRO AR 35241-26-0
 SOL 64-17-5 EtOH

RX(32) OF 55 ...AI ==> AS



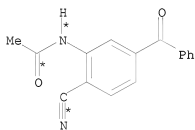
AI



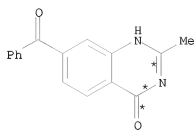
AS

RX(32) RCT AI 98012-93-2
 RGT E 7647-01-0 HCl
 PRO AS 98012-99-8
 SOL 64-17-5 EtOH

RX(33) OF 55 ...AJ ==> AT



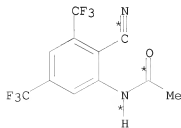
AJ



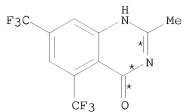
AT

RX(33) RCT AJ 98012-94-3
 RGT E 7647-01-0 HCl
 PRO AT 98013-00-4
 SOL 64-17-5 EtOH

RX(34) OF 55 ...AL ==> AU



AL



AU

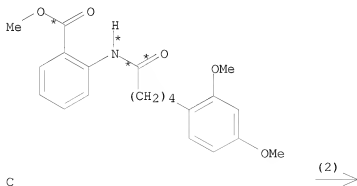
RX(34) RCT AL 98012-95-4
 RGT E 7647-01-0 HCl
 PRO AU 98013-01-5
 SOL 64-17-5 EtOH

L3 ANSWER 200 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 103:54028 CASREACT
 TITLE: Intramolecular reactions of N-nitrenes: oxidation of
 3-amino-2-(2,4-dimethoxyphenylbutyl)quinazolin-4(3H)-
 ones
 AUTHOR(S): Atkinson, Robert S.; Gawad, Nagwa A.
 CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999)
 (1985), (4), 825-30
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

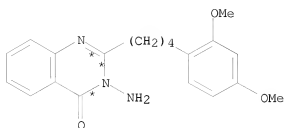
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The N-nitrenes generated by oxidation of the title compds. I (R = H, Me) were trapped by the remote 2,4-dimethoxyphenyl ring. Thus, oxidation of I (R = Me) by Pb(OAc)₄ in C₆H₆ gave 60% metacyclophane II, whereas oxidation in MeOH gave III, IV, and V; the structures of III and V were confirmed by x-ray anal. Oxidation of I (R = H) in MeOH and in C₆H₆ containing CH₂:CHCH₂OH gave VI and VII, resp. An explanation is given for the regiochem. of the trapping reaction.

RX(2) OF 35 ...C ==> E...



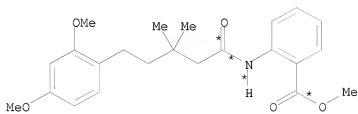
10/ 562,112



E

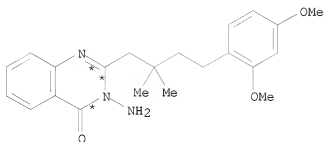
RX(2) RCT C 97305-81-2
 RGT F 302-01-2 N2H4
 PRO E 97305-82-3
 SOL 64-17-5 EtOH

RX(8) OF 35 ...T ==> U...



T

(8) \longrightarrow



U

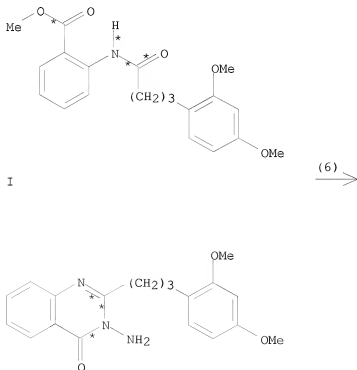
RX(8) RCT T 97305-85-6
 RGT F 302-01-2 N2H4
 PRO U 94922-06-2
 SOL 64-17-5 EtOH

L3 ANSWER 201 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 103:22566 CASREACT
 TITLE: Intramolecular reactions of N-nitrenes: oxidation of
 3-amino-2-(2,4-dimethoxyphenylpropyl)quinazolin-4(3H)-
 one
 AUTHOR(S): Atkinson, Robert S.; Gawad, Nagwa A.
 CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999)
 (1985), (2), 341-4
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

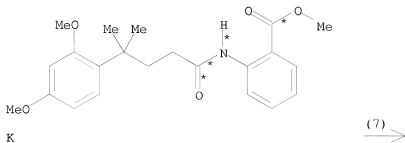
AB Oxidation of the title compound (I; R = H) or its di-Me analog I (R = Me) by
 Pb(OAc)₄ in MeOH containing K₂CO₃ for 5 min gave the corresponding tetracycles
 II (R = H, Me) in 29 and 55% yield, resp. On standing overnight in MeOH,
 II (R = H) was converted quant. to the cyclopentane ring-containing analog
 III, the structure of which was determined by x-ray anal.

RX(6) OF 40 ...I ==> Q...



RX(6) RCT I 96818-24-5
 RGT R 7803-57-8 N2H4-H2O
 PRO Q 87893-97-8
 SOL 64-17-5 EtOH

RX(7) OF 40 ...K ==> T...

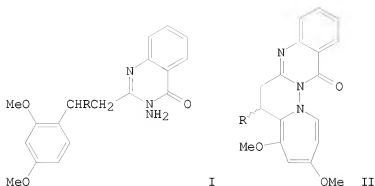


T

RX(7) RCT K 96818-25-6
 RGT R 7803-57-8 N2H4-H2O
 PRO T 87893-98-9
 SOL 64-17-5 EtOH

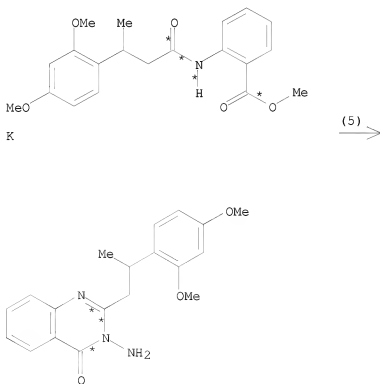
L3 ANSWER 202 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 103:22542 CASREACT
 TITLE: Intramolecular reactions of N-nitrenes: oxidation of
 3-amino-2-(2,4-dimethoxyphenylethyl)quinazolin-4(3H)-
 ones
 AUTHOR(S): Atkinson, Robert S.; Gawad, Nagwa A.
 CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999)
 (1985), (2), 335-9
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English

GI



AB Oxidation of the N-aminoquinazolones I (R = H, Me) by Pb(OAc)₄ in CHCl₃ for 5 min gave the corresponding 1H-azepines II [R = H (III), endo-Me (IV)]. Boat-to-boat flipping of the azepine ring in III is slow on the NMR time-scale, even at 140°. Heating IV in PhCl at 135° gave the corresponding stereoisomer II (R = exo-Me) with a min. free energy barrier of 30 kcal/mol. Reasons for the high barrier to azepine ring inversion are examined

RX(5) OF 33 ...K ==> L...

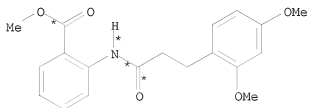


L

10/ 562,112

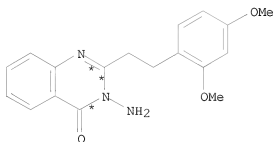
RX(5) RCT K 96818-14-3
 RGT M 7803-57-8 N2H4-H2O
 PRO L 92617-47-5
 SOL 64-17-5 EtOH

RX(6) OF 33 ...I ==> O...



I

(6) \Rightarrow

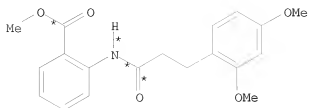


O

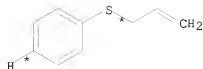
RX(6) RCT I 96818-15-4
 RGT M 7803-57-8 N2H4-H2O
 PRO O 92617-46-4
 SOL 64-17-5 EtOH

RX(19) OF 33 COMPOSED OF RX(6), RX(11)

RX(19) I + Z ==> AA

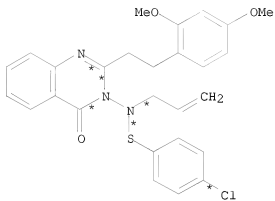


I



Z

2
STEPS
→

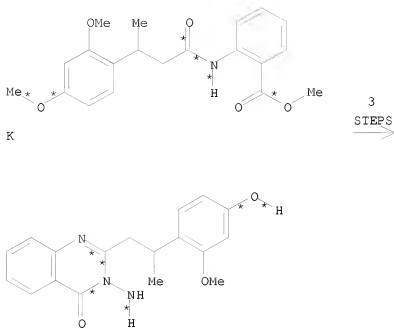


AA

RX(6) RCT I 96818-15-4
RGT M 7803-57-8 N2H4-H2O
PRO O 92617-46-4
SOL 64-17-5 EtOH

RX(11) RCT Z 5296-64-0, O 92617-46-4
RGT Q 546-67-8 Pb(OAc)4
PRO AA 92617-50-0
SOL 67-66-3 CHCl3

RX(31) OF 33 COMPOSED OF RX(5), RX(9), RX(10)
RX(31) K ==> V



V

RX(5) RCT K 96818-14-3
 RGT M 7803-57-8 N2H4-H2O
 PRO L 92617-47-5
 SOL 64-17-5 EtOH

RX(9) RCT L 92617-47-5
 RGT Q 546-67-8 Pb(OAc)4
 PRO T 96818-16-5
 SOL 67-56-1 MeOH

RX(10) RCT T 96818-16-5
 RGT W 7647-01-0 HCl, X 7440-66-6 Zn
 PRO V 96818-17-6
 SOL 67-56-1 MeOH, 7732-18-5 Water

L3 ANSWER 203 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:

102:220818 CASREACT

TITLE:

Possible antifertility agents. Part-I. Synthesis of
 2-(N,N-substituted-aminomethyl)-3-(2-pyridyl)-4(3H)-
 oxo-3,1-quinazolines
 Kulkarni, Y. D.; Abdi, S. H. R.; Sharma, V. L.
 Dep. Chem., Univ. Lucknow, Lucknow, 226 007, India
 Journal of the Indian Chemical Society (1984), 61(8),
 720-1

AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

CODEN: JICSAH; ISSN: 0019-4522

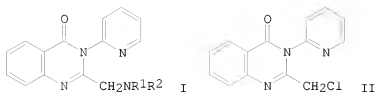
DOCUMENT TYPE:

Journal

LANGUAGE:

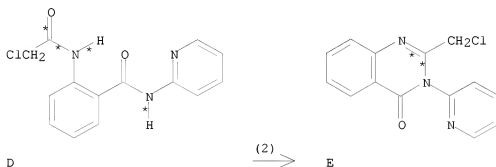
English

GI



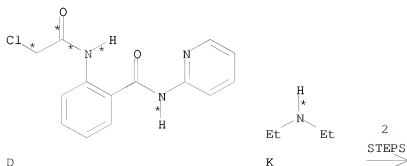
AB The title compds. I (NR₁R₂ = Et₂N, pyrrolidino, piperidino, 4-methylpiperidino, morpholino), potential contraceptives, were prepared in 5 steps from o-O₂NC₆H₄COCl and 2-aminopyridine via o-O₂NC₆H₄CONHR (R = 2-pyridyl), o-H₂NC₆H₄CONHR, o-ClCH₂CONHC₆H₄CONHR, and quinazolinone II. I showed little or no activity at 25 mg/kg animal (unidentified).

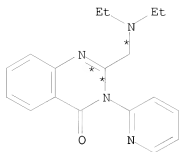
RX(2) OF 35 ...D ==> E...



RX(2) RCT D 96656-50-7
 PRO E 76535-05-2
 CAT 108-24-7 Ac2O

RX(11) OF 35 COMPOSED OF RX(2), RX(5)
 RX(11) D + K ==> L



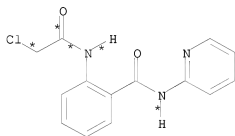


L

RX(2) RCT D 96656-50-7
 PRO E 76535-05-2
 CAT 108-24-7 Ac2O

RX(5) RCT E 76535-05-2, K 109-89-7
 PRO L 96656-51-8
 CAT 110-86-1 Pyridine

RX(12) OF 35 COMPOSED OF RX(2), RX(6)
 RX(12) D + N ==> O

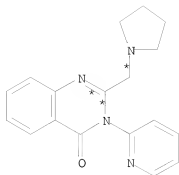


D



N

2
 STEPS
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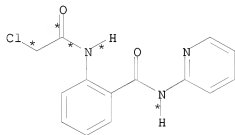
O

RX(2) RCT D 96656-50-7
 PRO E 76535-05-2
 CAT 108-24-7 Ac2O

RX(6) RCT E 76535-05-2, N 123-75-1
 PRO O 96656-52-9

RX(13) OF 35 COMPOSED OF RX(2), RX(7)

RX(13) D + P ==> Q

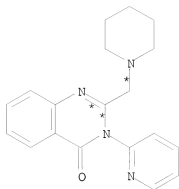


D



P

2
 STEPS
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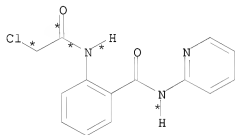


Q

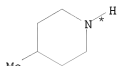
RX(2) RCT D 96656-50-7
 PRO E 76535-05-2
 CAT 108-24-7 Ac2O

RX(7) RCT E 76535-05-2, P 110-89-4
 PRO Q 96656-53-0

RX(14) OF 35 COMPOSED OF RX(2), RX(8)
 RX(14) D + R ==> S

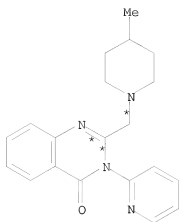


D



R

2
 STEPS
 →



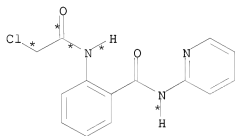
S

RX(2) RCT D 96656-50-7
 PRO E 76535-05-2
 CAT 108-24-7 Ac2O

RX(8) RCT E 76535-05-2, R 626-58-4
 PRO S 96656-54-1

RX(15) OF 35 COMPOSED OF RX(2), RX(9)

RX(15) D + T ==> U

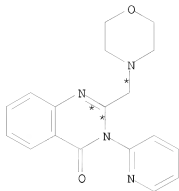


D



T

2
 STEPS
 →

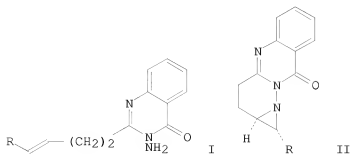


U

RX(2) RCT D 96656-50-7
PRO E 76535-05-2
CAT 108-24-7 Ac2O

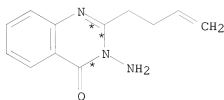
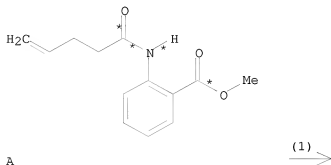
RX(9) RCT E 76535-05-2, T 110-91-8
PRO U 96656-55-2

L3 ANSWER 204 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 102:24574 CASREACT
TITLE: Intramolecular reactions of N-nitrenes with alkenes
AUTHOR(S): Atkinson, Robert S.; Malpass, John R.; Skinner, Karen L.; Woodthorpe, Katherine L.
CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1984), (8), 1905-12
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



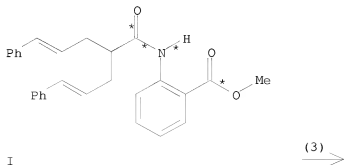
AB Oxidation of quinazolinones I (R = H, Ph) with Pb(OAc)₄ in CH₂Cl₂ gave the corresponding aziridines II in 50 and 76% yield, resp., through intramol. trapping of N-nitrenes by the double bond. Competitive intramol. trapping of the nitrene in 3-aminoquinazolinones with bifurcated chains at position 2 showed that these reactions are nonconcerted and occur via 7-membered transition states with the nitrene functioning as an electrophile.

RX(1) OF 21 ...A ==> B

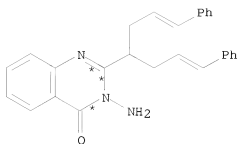


RX(1) RCT A 93681-77-7
 RGT C 302-01-2 N2H4
 PRO B 79091-40-0
 SOL 67-56-1 MeOH

RX(3) OF 21 ...I ==> J



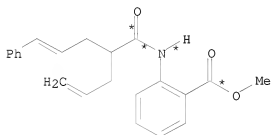
10/ 562,112



J
YIELD 65%

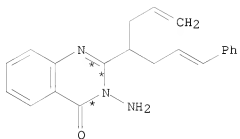
RX(3) RCT I 93681-78-8
 RGT C 302-01-2 N2H4
 PRO J 79091-43-3

RX(4) OF 21 ...K ==> L



K

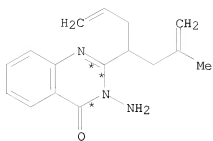
(4) →



L
YIELD 50%

RX(4) RCT K 93681-79-9
 RGT C 302-01-2 N2H4
 PRO L 79091-45-5

10/ 562,112

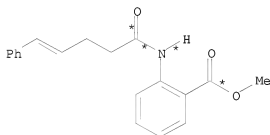


P

YIELD 73%

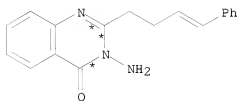
RX(6)	RCT	O 93681-81-3
	RGT	C 302-01-2 N2H4
	PRO	P 79091-47-7

RX(7) OF 21 ...Q ==> R



Q

(7) →

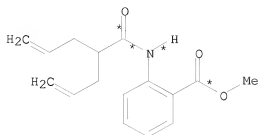


R

RX(7)	RCT	Q 93681-76-6
	RGT	C 302-01-2 N2H4
	PRO	R 79091-39-7
	SOL	67-56-1 MeOH

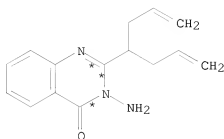
RX(13) OF 21 ...G ==> X

10/ 562,112



G

(13) →



X

YIELD 85%

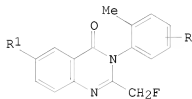
RX(13) RCT G 93698-03-4
RGT C 302-01-2 N2H4
PRO X 79091-44-4

L3 ANSWER 205 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 102:6537 CASREACT
TITLE: 2-Fluoromethyl-3-(2-methylphenyl)-6-amino-4(3H)-quinazolinones
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

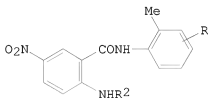
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 59128376	A	19840724	JP 1983-4707	19830113
JP 03004074	B	19910122		
EP 116268	A1	19840822	EP 1984-100011	19840102
EP 116268	B1	19880608		
R: BE, CH, DE, FR, GB, IT, LI, NL				
ZA 8400084	A	19840829	ZA 1984-84	19840105

CA 1218367	A1	19870224	CA 1984-445009	19840110
US 4714702	A	19871222	US 1986-888631	19860721
PRIORITY APPLN. INFO.:			JP 1983-4707	19830113
			US 1983-564006	19831221

OTHER SOURCE(S): MARPAT 102:6537
GI



I



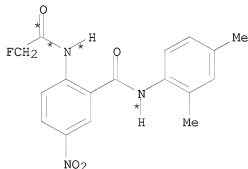
II

AB The title compds. (I; R = 4-Me, 4-Cl, 3-Me, 4-F, 4-Br, 4-MeO, 5-F, 5-Cl; R1 = H2N) were prepared by acylation of II (R2 = H) with FCH2COX (X = halo), cyclization of the resulting II (R2 = FCH2CO), and reduction of the resulting I (R1 = O2N). Thus, stirring 4 g II (R = 4-Me, R2 = H) with 2.18 g FCH2COCl in THF containing 2.36 g pyridine at room temperature gave 4.3 g II (R = 4-Me, R2 = FCH2CO), which (4 g) was heated with 3.5 g BF3-Et2O in AcOH at 100-105° to give 2.6 g I (R = 4-Me, R1 = O2N) (III). Reduction of 2 g III with SnCl2 in MeOH at room temperature gave 1.2 g I (R = 4-Me, R1 = H2N).

I

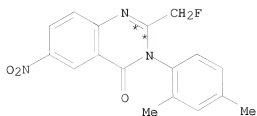
(R = 4-Cl) was a more potent muscle relaxant than mephesisin in mice.

RX(2) OF 4 D ==> E...



D

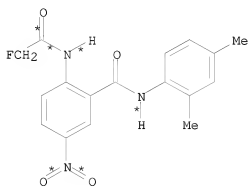
(2) →



E

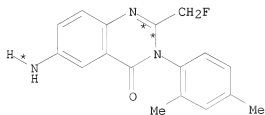
RX(2) RCT D 93670-44-1
PRO E 93670-45-2

RX(4) OF 4 COMPOSED OF RX(2), RX(3)
RX(4) D ==> F



D

2
STEPS
→

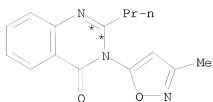


F

RX(2) RCT D 93670-44-1
PRO E 93670-45-2

RX(3) RCT E 93670-45-2
PRO F 93670-47-4

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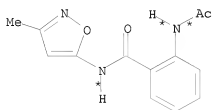


B

YIELD 28%

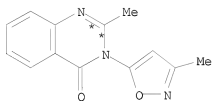
RX(1) RCT A 90059-30-6
RGT C 10025-87-3 POC13
PRO B 90059-38-4

RX(3) OF 30 ...F ==> G



F

(3) →

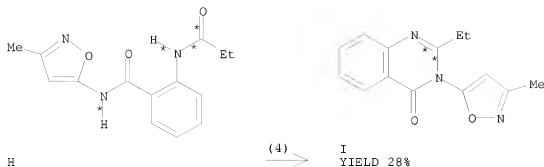


G

YIELD 28%

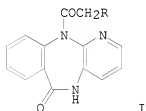
RX(3) RCT F 90059-29-3
RGT C 10025-87-3 POC13
PRO G 86134-19-2

RX(4) OF 30 ...H ==> I



RX(4) RCT H 344872-88-4
 RGT C 10025-87-3 POC13
 PRO I 86134-20-5

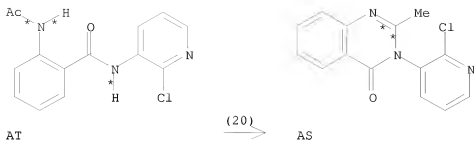
L3 ANSWER 207 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 100:34516 CASREACT
 TITLE: New synthesis of
 11-acyl-5,11-dihydro-6H-pyrido[2,3-
 b][1,4]benzodiazepin-6-ones and related studies
 AUTHOR(S): Kovac, T.; Oklobdzija, M.; Comisso, G.; Decorte, E.;
 Fajdiga, T.; Moimas, F.; Angeli, C.; Zonno, F.; Toso,
 R.; Sunjic, V.
 CORPORATE SOURCE: Chem. Res. Co., San Giovanni, Italy
 SOURCE: Journal of Heterocyclic Chemistry (1983), 20(5),
 1339-49
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB 11-Acyl-5,11-dihydro-6H-pyrido[2,3-b][1,4]benzodiazepin-6-ones I (R =
 4-methylpiperazino, imidazolo, 2-methylimidazolo) were prepared via
 N- α -chloroacetylation and aminolysis. Other attempts at cyclization
 to form I are also reported.

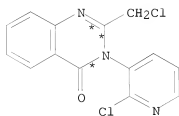
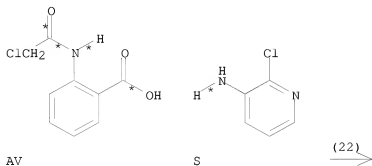
RX(20) OF 178 ...AT ==> AS...

10/ 562,112



RX(20) RCT AT 88369-52-2
PRO AS 20091-81-0

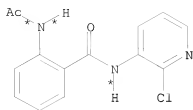
RX(22) OF 178 AV + S \implies AW...



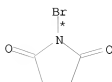
AW
YIELD 93%

RX(22) RCT AV 14422-49-2, S 6298-19-7
PRO AW 88369-53-3

RX(69) OF 178 COMPOSED OF RX(20), RX(23)
RX(69) AT + AX \implies AY

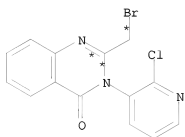


AT



AX

2
STEPS
→

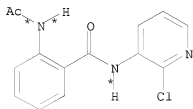


AY

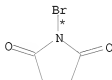
RX(20) RCT AT 88369-52-2
PRO AS 20091-81-0

RX(23) RCT AS 20091-81-0, AX 128-08-5
PRO AY 88369-54-4
CAT 78-67-1 AIBN

RX(70) OF 178 COMPOSED OF RX(20), RX(47)
RX(70) AT + 2 AX ==> BY

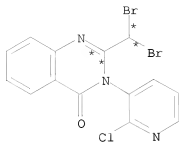


AT



2 AX

2
STEPS
→

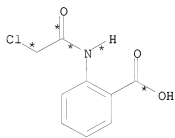


BY

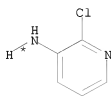
RX(20) RCT AT 88369-52-2
PRO AS 20091-81-0

RX(47) RCT AS 20091-81-0, AX 128-08-5
PRO BY 344868-00-4
CAT 78-67-1 AIBN

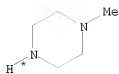
RX(72) OF 178 COMPOSED OF RX(22), RX(24)
RX(72) AV + S + AP ==> BA



AV

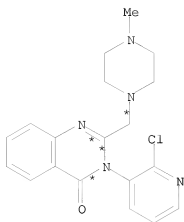


S



AP

2
STEPS
→

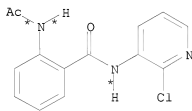


BA

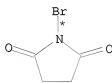
RX(22) RCT AV 14422-49-2, S 6298-19-7
PRO AW 88369-53-3

RX(24) RCT AW 88369-53-3, AP 109-01-3
PRO BA 88369-55-5

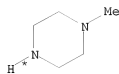
RX(110) OF 178 COMPOSED OF RX(20), RX(23), RX(25)
RX(110) AT + AX + AP ==> BA



AT

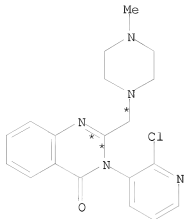


AX



AP

3
STEPS
=>



BA

YIELD 90%

RX(20) RCT AT 88369-52-2
PRO AS 20091-81-0

RX(23) RCT AS 20091-81-0, AX 128-08-5
PRO AY 88369-54-4
CAT 78-67-1 AIBN

RX(25) RCT AY 88369-54-4, AP 109-01-3
PRO BA 88369-55-5

L3 ANSWER 208 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 99:139890 CASREACT

TITLE: Synthesis of the metabolites of afloqualone and related compounds

AUTHOR(S): Yamada, Yoshihisa; Otsuka, Minezo; Tani, Junichi; Oine, Toyonari

CORPORATE SOURCE: Res. Lab. Appl. Biochem., Tanabe Seiyaku Co., Ltd., Osaka, 532, Japan

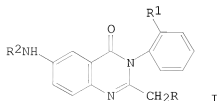
SOURCE: Chemical & Pharmaceutical Bulletin (1983), 31(4), 1158-65

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

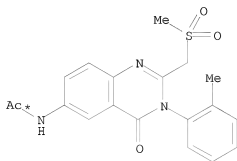
LANGUAGE: English

GI

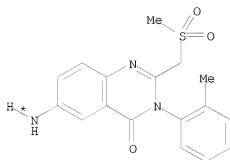


AB Seven main metabolites I [R = F, SMe, SO₂Me, SCH₂CH(NHAc)CO₂H, OH; R₁ = Me, CH₂OH; R₂ = Ac, COCH₂OH] of afloqualone (I, R = F, R₁ = Me, R₂ = H) and related 4(3H)-quinazolinone derivs. were synthesized. I (R = SMe, SO₂Me, R₁ = Me, R₂ = Ac) were prepared by the reaction of I (R = Cl, R₁ = Me, R₂ = Ac) with NaSMe followed by oxidation with H₂O₂. Reaction of I (R = Cl, R₁ = Me, R₂ = Ac) and N-acetylcysteine gave I [R = SCH₂CH(NHAc)CO₂H, R₁ = Me, R₂ = Ac]. Condensation of 2-fluoroacetamido-5-nitrobenzoic acid and 2-aminobenzyl alc. with dicyclohexylcarbodiimide in the presence of 1-hydroxybenzotriazole afforded 2-fluoromethyl-3-(o-hydroxymethylphenyl)-6-nitro-4(3H)-quinazolinone, which was converted to I (R = F, R₁ = CH₂OH, R₂ = Ac, COCH₂OH). Treatment of I (R = Br, R₁ = Me, R₂ = Ac) with AgBF₄·H₂O in Me₂SO gave I (R = OH, R₁ = Me, R₂ = Ac). None of the main metabolites showed significant central nervous system depressant activity.

RX(2) OF 41 ...E ==> F



E

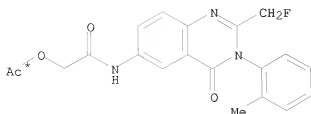


F

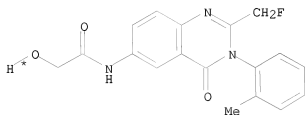
YIELD 69%

RX(2) RCT E 87266-00-0
RGT D 7647-01-0 HCl
PRO F 87266-03-3

RX(4) OF 41 ...I ==> J

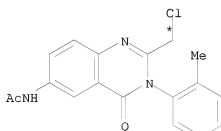


I

(4) \longrightarrow 

J

RX(4) RCT I 87265-98-3
 PRO J 87081-79-6
 CAT 144-55-8 NaHCO₃

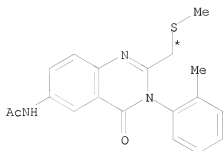
RX(6) OF 41 M + N \implies O...

M



N

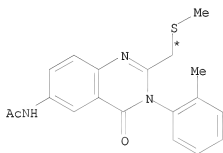
(6) \longrightarrow



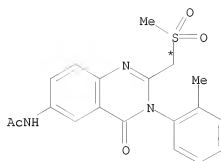
O
YIELD 92%

RX(6) RCT M 61899-78-3, N 5188-07-8
PRO O 87265-99-4

RX(7) OF 41 ...O ==> E...



O

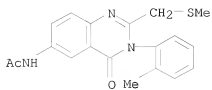


E
YIELD 48%

RX(7) RCT O 87265-99-4
RGT P 7722-84-1 H2O2
PRO E 87266-00-0

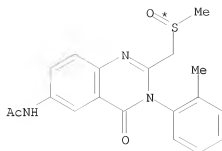
RX(8) OF 41 ...O ==> Q

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O

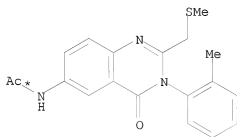
(8)



Q
YIELD 91%

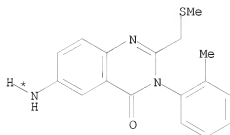
RX(8) RCT O 87265-99-4
 RGT P 7722-84-1 H2O2
 PRO Q 87266-01-1

RX(9) OF 41 ...O ==> R...



O

(9)



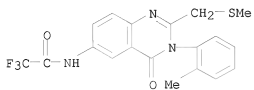
R
YIELD 90%

RX(9) RCT O 87265-99-4
 RGT D 7647-01-0 HCl

10/ 562,112

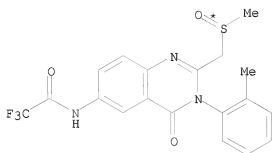
PRO R 87266-02-2

RX(11) OF 41 ...T ==> U...



T

(11)

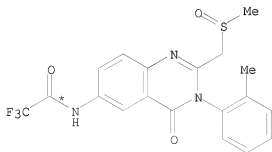


U

YIELD 77%

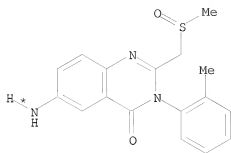
RX(11) RCT T 87266-05-5
RGT P 7722-84-1 H2O2
PRO U 87266-06-6

RX(12) OF 41 ...U ==> V



U

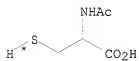
(12)



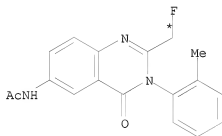
V

RX(12) RCT U 87266-06-6
 PRO V 87266-07-7
 CAT 67-56-1 MeOH

RX(13) OF 41 X + Y ==> Z...



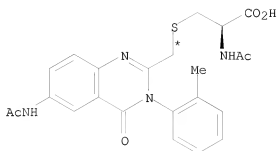
X



Y

(13)

10/ 562,112

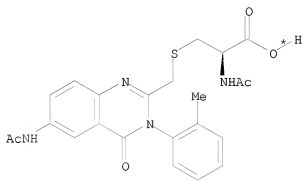


Z

YIELD 92%

RX(13) RCT X 616-91-1, Y 61899-79-4
PRO Z 87266-09-9

RX(14) OF 41 ...Z + AA ==> AB



Z

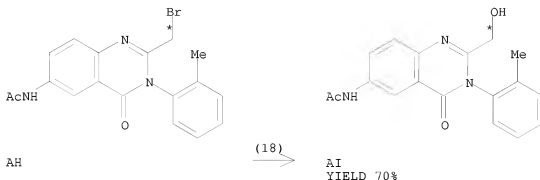


AA

(14) →

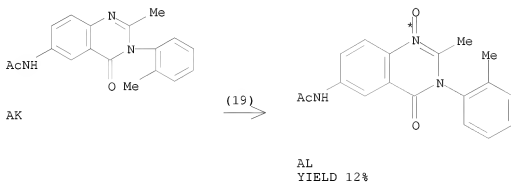
PRO A 87266-11-3

RX(18) OF 41 AH ==> AI



RX(18) RCT AH 87266-12-4
 RGT AJ 14104-20-2 AgBF₄
 PRO AI 87266-13-5

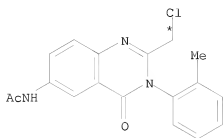
RX(19) OF 41 AK ==> AL



RX(19) RCT AK 1096-46-4
 RGT P 7722-84-1 H₂O₂
 PRO AL 87266-14-6

RX(24) OF 41 COMPOSED OF RX(6), RX(7)
 RX(24) M + N ==> E

10/ 562,112

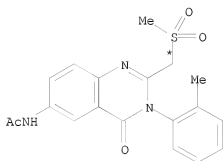


M



N

2
STEPS
→



E

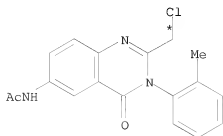
YIELD 48%

RX(6) RCT M 61899-78-3, N 5188-07-8
PRO O 87265-99-4

RX(7) RCT O 87265-99-4
RGT P 7722-84-1 H2O2
PRO E 87266-00-0

RX(25) OF 41 COMPOSED OF RX(6), RX(8)

RX(25) M + N ==> Q

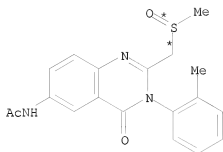


M



N

2
STEPS
→

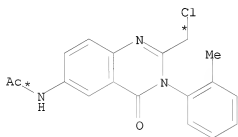


Q
YIELD 91%

RX(6) RCT M 61899-78-3, N 5188-07-8
PRO O 87265-99-4

RX(8) RCT O 87265-99-4
RGT P 7722-84-1 H2O2
PRO Q 87266-01-1

RX(26) OF 41 COMPOSED OF RX(6), RX(9)
RX(26) M + N ==> R



M

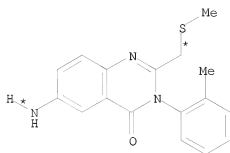


● Na

N

2
STEPS
→

10/ 562,112



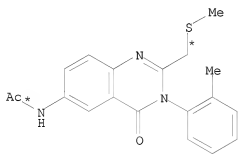
R

YIELD 90%

RX(6) RCT M 61899-78-3, N 5188-07-8
PRO O 87265-99-4

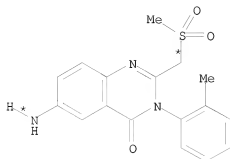
RX(9) RCT O 87265-99-4
RGT D 7647-01-0 HCl
PRO R 87266-02-2

RX(27) OF 41 COMPOSED OF RX(7), RX(2)
RX(27) O ==> F



O

2
STEPS
→

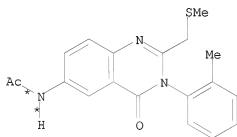


F
YIELD 69%

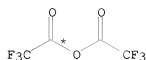
RX(7) RCT O 87265-99-4
RGT P 7722-84-1 H2O2
PRO E 87266-00-0

RX(2) RCT E 87266-00-0
RGT D 7647-01-0 HCl
PRO F 87266-03-3

RX(28) OF 41 COMPOSED OF RX(9), RX(10)
RX(28) O + S ==> T

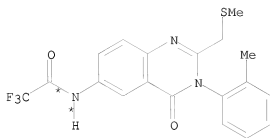


O



S

2
STEPS
→

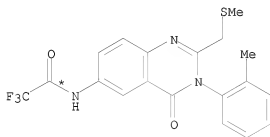


T
YIELD 95%

RX(9) RCT O 87265-99-4
RGT D 7647-01-0 HCl
PRO R 87266-02-2

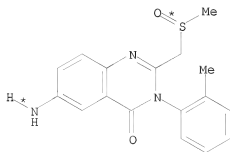
RX(10) RCT R 87266-02-2, S 407-25-0
PRO T 87266-05-5

RX(30) OF 41 COMPOSED OF RX(11), RX(12)
RX(30) T ==> V



T

2
STEPS
→



V

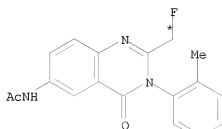
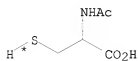
10/ 562,112

RX(11) RCT T 87266-05-5
RGT P 7722-84-1 H2O2
PRO U 87266-06-6

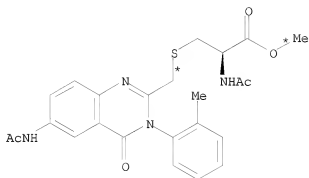
RX(12) RCT U 87266-06-6
PRO V 87266-07-7
CAT 67-56-1 MeOH

RX(31) OF 41 COMPOSED OF RX(13), RX(14)

RX(31) X + Y + AA ==> AB



2
STEPS
=>



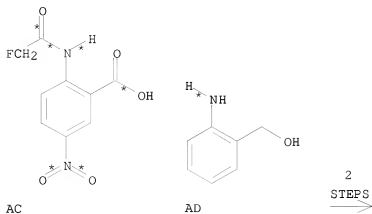
AB
YIELD 87%

RX(13) RCT X 616-91-1, Y 61899-79-4
PRO Z 87266-09-9

RX(14) RCT Z 87266-09-9, AA 334-88-3
PRO AB 87266-08-8

RX(32) OF 41 COMPOSED OF RX(15), RX(1)

RX(32) AC + AD ==> B

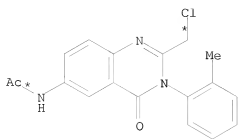
B
YIELD 64%

RX(15) RCT AC 87266-10-2, AD 5344-90-1
 PRO A 87266-11-3

RX(1) RCT A 87266-11-3
 RGT C 7772-99-8 SnCl₂, D 7647-01-0 HCl
 PRO B 73832-13-0

RX(33) OF 41 COMPOSED OF RX(6), RX(7), RX(2)

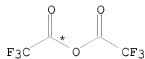
RX(33) M + N ==> F



M

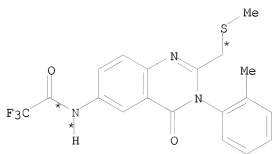


N



S

3
STEPS
→



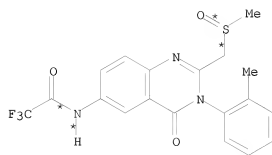
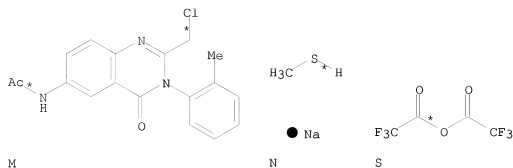
T
YIELD 95%

RX(6) RCT M 61899-78-3, N 5188-07-8
PRO O 87265-99-4

RX(9) RCT O 87265-99-4
RGT D 7647-01-0 HCl
PRO R 87266-02-2

RX(10) RCT R 87266-02-2, S 407-25-0
PRO T 87266-05-5

RX(35) OF 41 COMPOSED OF RX(9), RX(10), RX(11)
RX(35) O + S ==> U



YIELD 77%

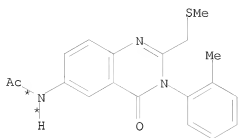
RX(6) RCT M 61899-78-3, N 5188-07-8
PRO O 87265-99-4

RX(9) RCT O 87265-99-4
RGT D 7647-01-0 HCl
PRO R 87266-02-2

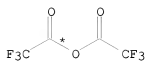
RX(10) RCT R 87266-02-2, S 407-25-0
PRO T 87266-05-5

RX(11) RCT T 87266-05-5
RGT P 7722-84-1 H2O2
PRO U 87266-06-6

RX(38) OF 41 COMPOSED OF RX(9), RX(10), RX(11), RX(12)
RX(38) O + S ==> V

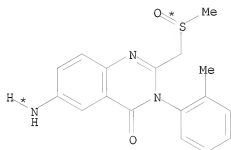


O



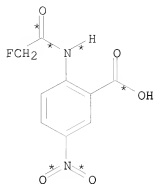
S

4
STEPS
→

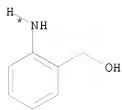


V

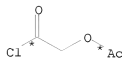
RX(9)	RCT	O	87265-99-4
	RGT	D	7647-01-0 HCl
	PRO	R	87266-02-2
RX(10)	RCT	R	87266-02-2, S 407-25-0
	PRO	T	87266-05-5
RX(11)	RCT	T	87266-05-5
	RGT	P	7722-84-1 H2O2
	PRO	U	87266-06-6
RX(12)	RCT	U	87266-06-6
	PRO	V	87266-07-7
	CAT	67-56-1	MeOH
RX(39)	OF	41	COMPOSED OF RX(15), RX(1), RX(16)
RX(39)	AC	+	AD + AE ==> AF



AC

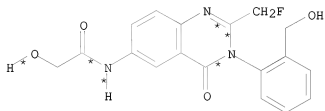


AD



G

3
STEPS
→



AG

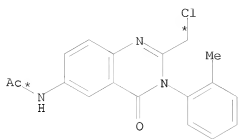
YIELD 70%

RX(15) RCT AC 87266-10-2, AD 5344-90-1
PRO A 87266-11-3

RX(1) RCT A 87266-11-3
RGT C 7772-99-8 SnCl2, D 7647-01-0 HCl
PRO B 73832-13-0

RX(17) RCT G 13831-31-7, B 73832-13-0
PRO AG 87081-80-9

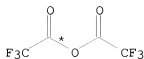
RX(41) OF 41 COMPOSED OF RX(6), RX(9), RX(10), RX(11), RX(12)
RX(41) M + N + S ==> V



M

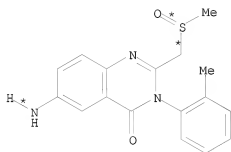


N



S

5
STEPS
→



V

RX(6) RCT M 61899-78-3, N 5188-07-8
PRO O 87265-99-4

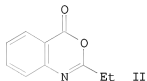
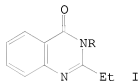
RX(9) RCT O 87265-99-4
RGT D 7647-01-0 HCl
PRO R 87266-02-2

RX(10) RCT R 87266-02-2, S 407-25-0
PRO T 87266-05-5

RX(11) RCT T 87266-05-5
RGT P 7722-84-1 H2O2
PRO U 87266-06-6

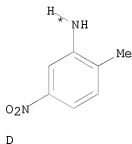
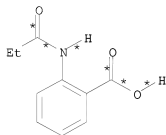
RX(12) RCT U 87266-06-6
PRO V 87266-07-7
CAT 67-56-1 MeOH

L3 ANSWER 209 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 98:198154 CASREACT
 TITLE: Synthesis and properties of
 2-ethyl-3-aryl(arylamino)-4(3H)-quinazolinones
 AUTHOR(S): Smirnova, N. N.; Kozhevnikov, Yu. V.
 CORPORATE SOURCE: Perm. Gos. Farm. Inst., Perm, USSR
 SOURCE: Deposited Doc. (1982), VINITI 1613-82, 7 pp. Avail.:
 VINITI
 DOCUMENT TYPE: Report
 LANGUAGE: Russian
 GI

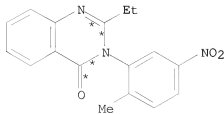


AB The title compds. I [R = 2,5-Me(O₂N)C₆H₃, 2,4-(O₂N)MeC₆H₃, 2,5-Me₂C₆H₃, PhNH, o-, m-, p-MeC₆H₄NH, p-BrC₆H₄NH] were prepared in 25-75% yields by cyclocondensation of II with RNH₂.

RX(10) OF 17 COMPOSED OF RX(1), RX(2)
 RX(10) A + D ==> E



2
 STEPS
 →



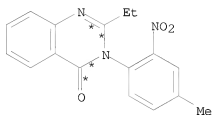
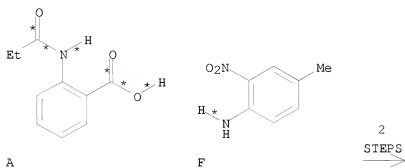
E
 YIELD 64%

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RX(1) RCT A 19165-26-5
 PRO B 2916-09-8
 CAT 75-07-0 MeCHO

RX(2) RCT B 2916-09-8, D 99-55-8
 PRO E 85731-86-8

RX(11) OF 17 COMPOSED OF RX(1), RX(3)
 RX(11) A + F ==> G

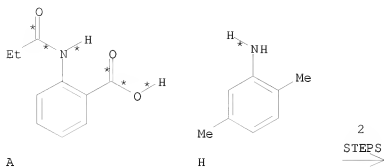


G
 YIELD 25%

RX(1) RCT A 19165-26-5
 PRO B 2916-09-8
 CAT 75-07-0 MeCHO

RX(3) RCT B 2916-09-8, F 89-62-3
 PRO G 85731-87-9

RX(12) OF 17 COMPOSED OF RX(1), RX(4)
 RX(12) A + H ==> I

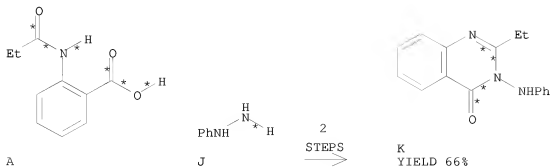


I
YIELD 37%

RX(1) RCT A 19165-26-5
PRO B 2916-09-8
CAT 75-07-0 MeCHO

RX(4) RCT B 2916-09-8, H 95-78-3
PRO I 85731-88-0

RX(13) OF 17 COMPOSED OF RX(1), RX(5)
RX(13) A + J ==> K



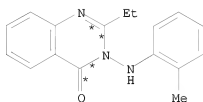
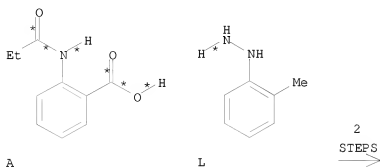
RX(1) RCT A 19165-26-5
PRO B 2916-09-8

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CAT 75-07-0 MeCHO

RX(5) RCT B 2916-09-8, J 100-63-0
PRO K 50547-52-9

RX(14) OF 17 COMPOSED OF RX(1), RX(6)
RX(14) A + L ==> M

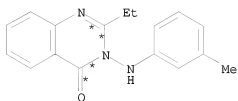
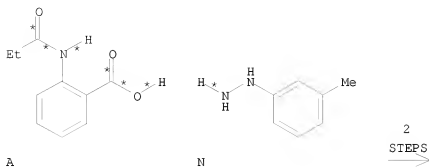


M
YIELD 75%

RX(1) RCT A 19165-26-5
PRO B 2916-09-8
CAT 75-07-0 MeCHO

RX(6) RCT B 2916-09-8, L 529-27-1
PRO M 85731-89-1

RX(15) OF 17 COMPOSED OF RX(1), RX(7)
RX(15) A + N ==> O

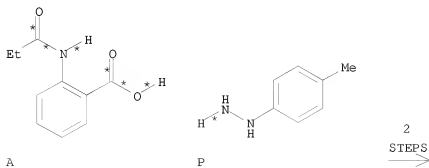


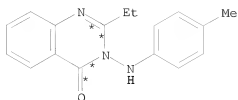
O
YIELD 40%

RX(1) RCT A 19165-26-5
PRO B 2916-09-8
CAT 75-07-0 MeCHO

RX(7) RCT B 2916-09-8, N 536-89-0
PRO O 85731-90-4

RX(16) OF 17 COMPOSED OF RX(1), RX(8)
RX(16) A + P ==> Q



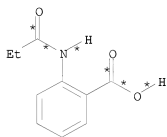


Q
YIELD 43%

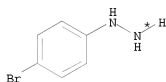
RX(1) RCT A 19165-26-5
PRO B 2916-09-8
CAT 75-07-0 MeCHO

RX(8) RCT B 2916-09-8, P 539-44-6
PRO Q 85731-91-5

RX(17) OF 17 COMPOSED OF RX(1), RX(9)
RX(17) A + R ==> S

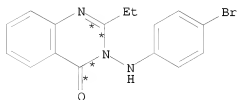


A



R

2
STEPS
→



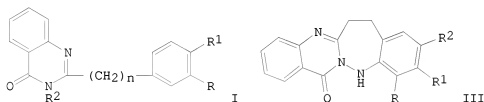
S
YIELD 44%

RX(1) RCT A 19165-26-5
PRO B 2916-09-8
CAT 75-07-0 MeCHO

RX(9) RCT B 2916-09-8, R 589-21-9

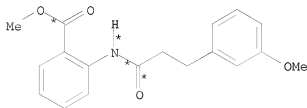
PRO S 85731-92-6

L3 ANSWER 210 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 98:16656 CASREACT
 TITLE: Intramolecular reactions of N-nitrenes: oxidation of
 3-amino-2-(arylalkyl)quinazolin-4(3H)-ones
 AUTHOR(S): Atkinson, Robert S.; Malpass, John R.; Woodthorpe,
 Katherine L.
 CORPORATE SOURCE: Dep. Chem., Univ. Leicester, Leicester, LE1 7RH, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999)
 (1982), (10), 2407-12
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



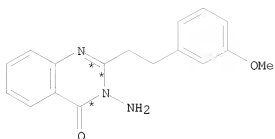
AB Oxidation of quinazolines I ($R = \text{OMe}$; $R_1 = \text{H}$, OMe ; $R_2 = \text{NH}_2$; $n = 2$) with $\text{Pd}(\text{OAc})_4$ in CH_2Cl_2 at room temperature gave I (same R , R_1 , n ; $R_2 = \text{H}$) (II) and the diazepines III ($R = \text{H}$, OMe ; $R_1 \neq R_2 = \text{H}$, OMe) via the corresponding N-nitrene intermediates. On oxidation under analogous conditions I ($n = 2$, $R = \text{H}$, $R_1 = \text{OMe}$; $n = 1$, $R \neq R_1 = \text{H}$, OMe ; $R_2 = \text{NH}_2$) gave only the deamination products II. Azepine formation involves electrophilic aromatic substitution by the nitrene on the aromatic ring via a 7-membered transition state.

RX(4) OF 38 ...H ==> I...



H

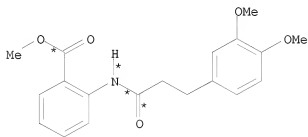
(4) →



I

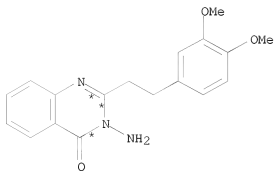
RX(4) RCT H 83988-42-5
 RGT J 302-01-2 N2H4
 PRO I 78649-10-2
 SOL 67-56-1 MeOH

RX(5) OF 38 ...L ==> M



L

(5)



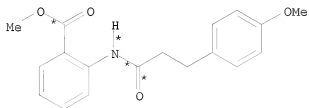
M

RX(5) RCT L 59282-10-9
 RGT J 302-01-2 N2H4

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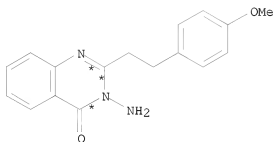
PRO M 78649-11-3
SOL 67-56-1 MeOH

RX(6) OF 38 ...N ==> O...



N

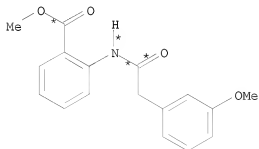
(6)
→



O

RX(6) RCT N 83988-43-6
RGT J 302-01-2 N2H4
PRO O 78649-12-4
SOL 67-56-1 MeOH

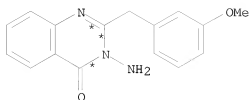
RX(7) OF 38 ...P ==> Q



P

(7)
→

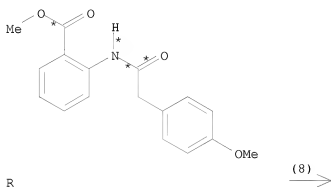
10/ 562,112



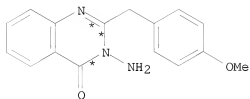
Q

RX(7) RCT P 83988-44-7
 RGT J 302-01-2 N2H4
 PRO Q 83988-47-0
 SOL 67-56-1 MeOH

RX(8) OF 38 ...R ==> S



R

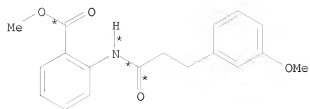


S

RX(8) RCT R 83988-45-8
 RGT J 302-01-2 N2H4
 PRO S 83988-46-9
 SOL 67-56-1 MeOH

RX(21) OF 38 COMPOSED OF RX(4), RX(9)
 RX(21) H + T ==> U

10/ 562,112

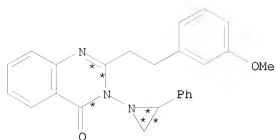


H



T

2
STEPS
→

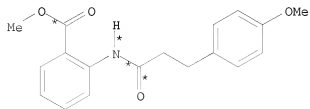


U

RX (4) RCT H 83988-42-5
 RGT J 302-01-2 N2H4
 PRO I 78649-10-2
 SOL 67-56-1 MeOH

RX (9) RCT I 78649-10-2, T 100-42-5
 PRO U 78649-18-0
 SOL 75-09-2 CH2Cl2

RX (22) OF 38 COMPOSED OF RX (6), RX (10)
RX (22) N + T ==> W

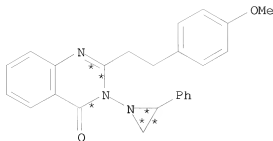


N



T

2
STEPS
→

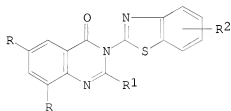


W

RX(6) RCT N 83988-43-6
 RGT J 302-01-2 N2H4
 PRO O 78649-12-4
 SOL 67-56-1 MeOH

RX(10) RCT O 78649-12-4, T 100-42-5
 PRO W 78649-19-1
 SOL 75-09-2 CH2Cl2

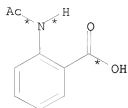
L3 ANSWER 211 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 97:72319 CASREACT
 TITLE: Synthesis of some new 4(3H)-quinazolinones as
 potential CNS depressants
 AUTHOR(S): Chaurasia, M. Ram; Sharma, Surendra K.
 CORPORATE SOURCE: Dep. Chem., D.A.V.(P.G.) Coll., Dehra Dun, India
 SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1982),
 315(4), 377-81
 CODEN: ARPMA5; ISSN: 0365-6233
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



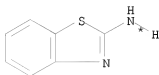
I

AB Quinazolinones I (R = H, Br, R1 = Me, styryl; R2 = H, Me, Cl, OMe, Et, Br in 4-, 5-, or 6-positions) were prepared by condensing the appropriate N-acetylanthranilic acid with 2-aminobenzothiazoles in the presence PC13 (4 h in refluxing toluene) followed by optional reaction with benzaldehyde. Five I were tested for CNS depressant activity in mice and found to be active.

RX(1) OF 34 A + B ==> C

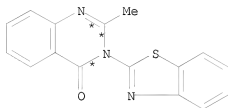


A



B

(1) →

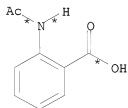


C

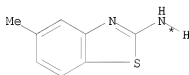
YIELD 51%

RX(1) RCT A 89-52-1, B 136-95-8
 RGT D 7719-12-2 PC13
 PRO C 81762-52-9

RX(2) OF 34 A + E ==> F



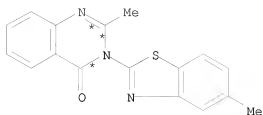
A



E

(2) →

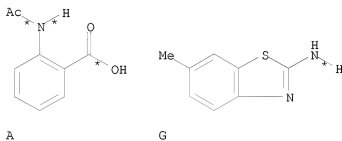
10/ 562,112



F
YIELD 45%

RX(2) RCT A 89-52-1, E 14779-17-0
RGT D 7719-12-2 PC13
PRO F 81762-54-1

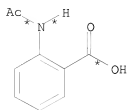
RX(3) OF 34 A + G ==> H



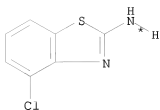
H
YIELD 49%

RX(3) RCT A 89-52-1, G 2536-91-6
RGT D 7719-12-2 PC13
PRO H 81762-55-2

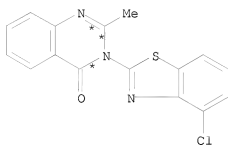
RX(4) OF 34 A + I ==> J



A



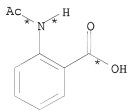
I

(4) \longrightarrow 

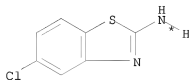
J

YIELD 35%

RX(4) RCT A 89-52-1, I 19952-47-7
 RGT D 7719-12-2 PC13
 PRO J 81762-56-3

RX(5) OF 34 A + K \implies L

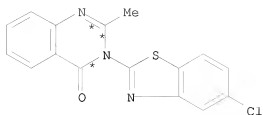
A



K

(5) \longrightarrow

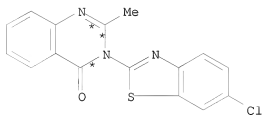
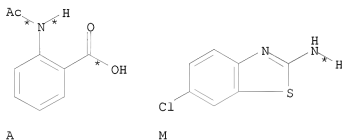
10/ 562,112



L
YIELD 48%

RX(5) RCT A 89-52-1, K 20358-00-3
RGT D 7719-12-2 PC13
PRO L 81762-57-4

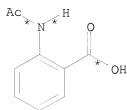
RX(6) OF 34 A + M ==> N...



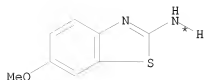
N
YIELD 36%

RX(6) RCT A 89-52-1, M 95-24-9
RGT D 7719-12-2 PC13
PRO N 81762-58-5

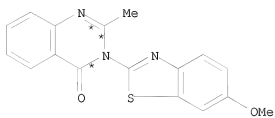
RX(7) OF 34 A + O ==> P



A



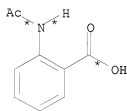
O

(7) \Rightarrow 

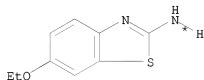
P

YIELD 32%

RX(7) RCT A 89-52-1, O 1747-60-0
 RGT D 7719-12-2 PC13
 PRO P 81762-60-9

RX(8) OF 34 A + Q \Rightarrow R...

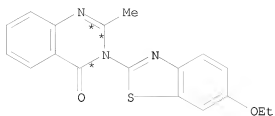
A



Q

(8) \Rightarrow

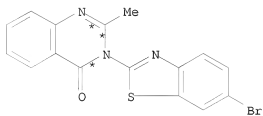
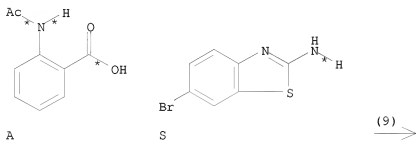
10/ 562,112



R
YIELD 74%

RX(8) RCT A 89-52-1, Q 94-45-1
RGT D 7719-12-2 PC13
PRO R 81762-61-0

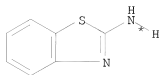
RX(9) OF 34 A + S ==> T



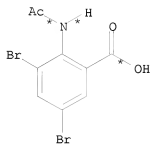
T
YIELD 52%

RX(9) RCT A 89-52-1, S 15864-32-1
RGT D 7719-12-2 PC13
PRO T 81797-04-8

RX(10) OF 34 B + U ==> V

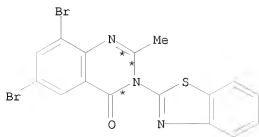


B



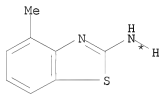
U

(10)

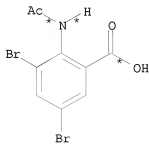
V
YIELD 60%

RX(10) RCT B 136-95-8, U 16610-45-0
RGT D 7719-12-2 PC13
PRO V 81762-62-1

RX(11) OF 34 W + U ==> X



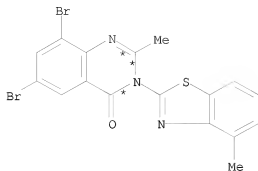
W



U

(11)

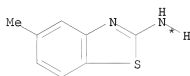
10/ 562,112



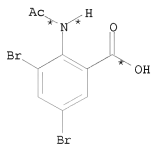
X
YIELD 42%

RX(11) RCT W 1477-42-5, U 16610-45-0
RGT D 7719-12-2 PC13
PRO X 81762-63-2

RX(12) OF 34 E + U ==> Y

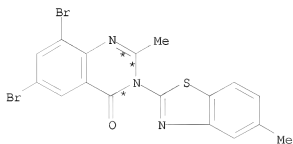


E



U

(12) →



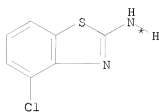
Y
YIELD 51%

RX(12) RCT E 14779-17-0, U 16610-45-0

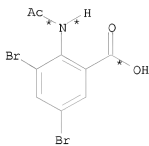
10/ 562,112

PRO Y 81762-64-3

RX(13) OF 34 I + U ==> Z

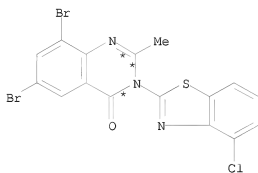


I



U

(13) 



Z

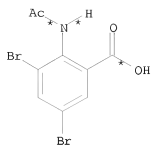
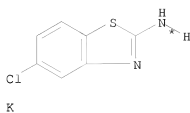
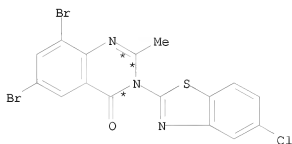
YIELD 58%

RX(13) RCT I 19952-47-7, U 16610-45-0

RGT D 7719-12-2 PC13

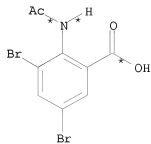
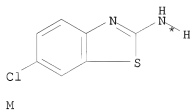
PRO Z 81762-66-5

RX(14) OF 34 K + U ==> AA

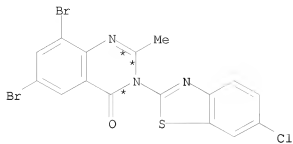
(14) \longrightarrow 

YIELD 62%

RX(14) RCT K 20358-00-3, U 16610-45-0
 RGT D 7719-12-2 PC13
 PRO AA 81762-67-6

RX(15) OF 34 M + U \implies AB...(15) \longrightarrow

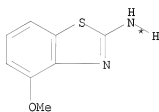
10/ 562,112



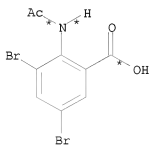
AB
YIELD 49%

RX(15) RCT M 95-24-9, U 16610-45-0
RGT D 7719-12-2 PC13
PRO AB 81762-68-7

RX(16) OF 34 AC + U ==> AD...

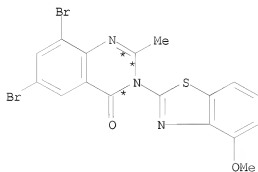


AC



U

(16) \longrightarrow



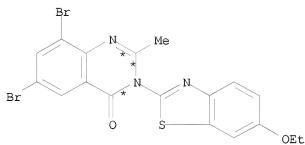
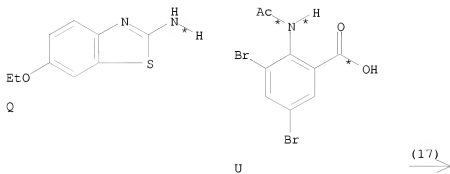
AD
YIELD 46%

RX(16) RCT AC 5464-79-9, U 16610-45-0

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RGT D 7719-12-2 PC13
PRO AD 81762-69-8

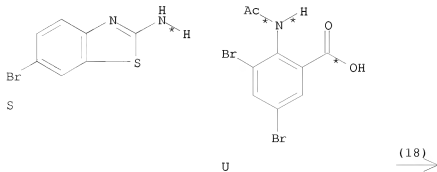
RX(17) OF 34 Q + U ==> AE



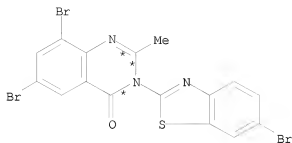
AE
YIELD 61%

RX(17) RCT Q 94-45-1, U 16610-45-0
RGT D 7719-12-2 PC13
PRO AE 81762-71-2

RX(18) OF 34 S + U ==> AF



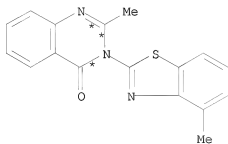
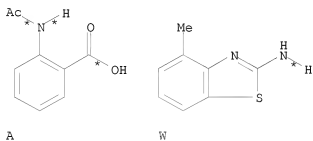
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AF
YIELD 59%

RX(18) RCT S 15864-32-1, U 16610-45-0
 RGT D 7719-12-2 PC13
 PRO AF 81762-72-3

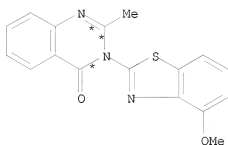
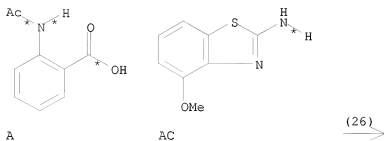
RX(25) OF 34 A + W ==> AG...



AG
YIELD 55%

RX(25) RCT A 89-52-1, W 1477-42-5
 RGT D 7719-12-2 PC13
 PRO AG 81762-53-0

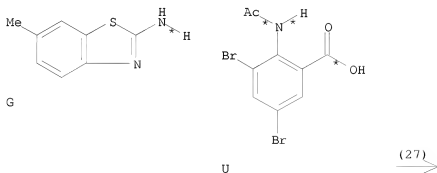
RX(26) OF 34 A + AC ==> AP



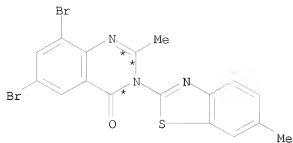
YIELD 31%

RX(26) RCT A 89-52-1, AC 5464-79-9
 RGT D 7719-12-2 PC13
 PRO AP 81762-59-6

RX(27) OF 34 G + U ==> AL...



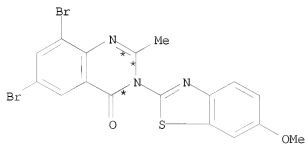
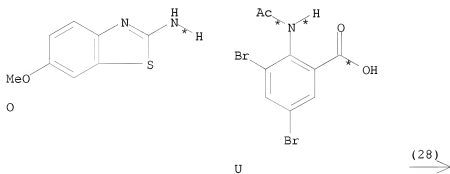
10/ 562,112



AL
YIELD 52%

RX(27) RCT G 2536-91-6, U 16610-45-0
RGT D 7719-12-2 PC13
PRO AL 81762-65-4

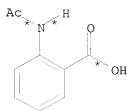
RX(28) OF 34 O + U ==> AQ



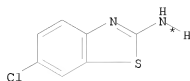
AQ
YIELD 56%

RX(28) RCT O 1747-60-0, U 16610-45-0
RGT D 7719-12-2 PC13
PRO AQ 81762-70-1

RX(29) OF 34 COMPOSED OF RX(6), RX(20)
 RX(29) A + M + AH ==> AJ



A

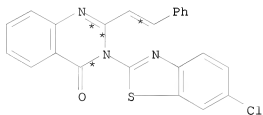


M



AH

2
STEPS
→

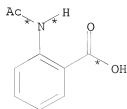


AJ
 YIELD 65%

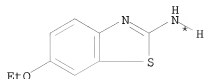
RX(6) RCT A 89-52-1, M 95-24-9
 RGT D 7719-12-2 PC13
 PRO N 81762-58-5

RX(20) RCT N 81762-58-5, AH 100-52-7
 PRO AJ 344572-35-6

RX(30) OF 34 COMPOSED OF RX(8), RX(21)
 RX(30) A + Q + AH ==> AK



A



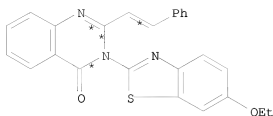
Q



AH

2
STEPS
→

10/ 562,112

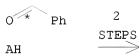
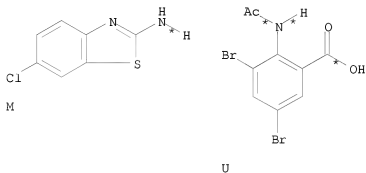


AK
YIELD 61%

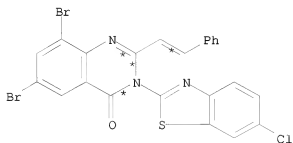
RX(8) RCT A 89-52-1, Q 94-45-1
RGT D 7719-12-2 PC13
PRO R 81762-61-0

RX(21) RCT R 81762-61-0, AH 100-52-7
PRO AK 344586-30-7

RX(31) OF 34 COMPOSED OF RX(15), RX(23)
RX(31) M + U + AH ==> AN



2
STEPS
→



AN
YIELD 69%

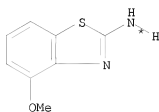
RX(15) RCT M 95-24-9, U 16610-45-0
RGT D 7719-12-2 PC13

10/ 562,112

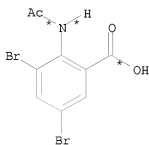
PRO AB 81762-68-7

RX(23) RCT AB 81762-68-7, AH 100-52-7
PRO AN 344586-29-4

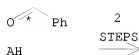
RX(32) OF 34 COMPOSED OF RX(16), RX(24)
RX(32) AC + U + AH ==> AO



AC

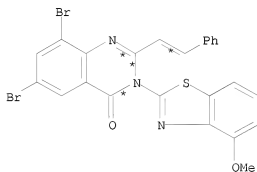


U



AH

2
STEPS
→



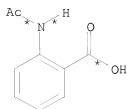
AO

YIELD 49%

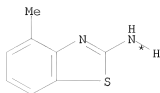
RX(16) RCT AC 5464-79-9, U 16610-45-0
RGT D 7719-12-2 PC13
PRO AD 81762-69-8

RX(24) RCT AD 81762-69-8, AH 100-52-7
PRO AO 344587-22-0

RX(33) OF 34 COMPOSED OF RX(25), RX(19)
RX(33) A + W + AH ==> AI



A

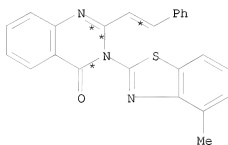


W



AH

2
STEPS
→



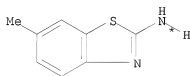
AI

YIELD 71%

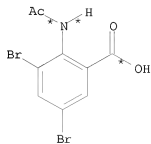
RX(25) RCT A 89-52-1, W 1477-42-5
RGT D 7719-12-2 PC13
PRO AG 81762-53-0

RX(19) RCT AG 81762-53-0, AH 100-52-7
PRO AI 344572-36-7

RX(34) OF 34 COMPOSED OF RX(27), RX(22)
RX(34) G + U + AH ==> AM



G

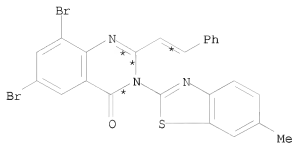


U



AH

2
STEPS
→

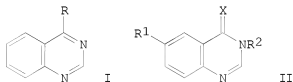


AM
YIELD 59%

RX(27) RCT G 2536-91-6, U 16610-45-0
RGT D 7719-12-2 PC13
PRO AL 81762-65-4

RX(22) RCT AL 81762-65-4, AH 100-52-7
PRO AM 344586-28-3

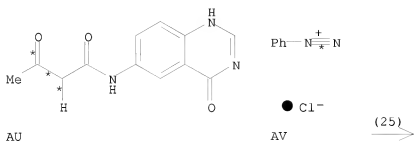
L3 ANSWER 212 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 97:55767 CASREACT
TITLE: Some reactions of 4-chloroquinazoline, 6-nitro- and
6-amino-4(3H)-quinazolones
AUTHOR(S): Anwar, M.; Abdel-Hay, F. I.; Elbarbary, A. A.;
El-Borai, M.
CORPORATE SOURCE: Fac. Sci., Tanta Univ., Tanta, Egypt
SOURCE: Revue Roumaine de Chimie (1981), 26(11-12), 1469-78
CODEN: RRCHAX; ISSN: 0035-3930
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Quinazolines I [R = NHCONH₂, NHCHO, NHAc, NAcPh, NAcC₆H₄Me-2, NAcC₆H₄Me-4, N-acetyl-N-1-naphthylamino, NHHNC₆H₄NO₂-4, NHHNC₆H₃(NO₂)₂-2,4] were prepared by aminating I (R = Cl). II (X = O, S; R₁ = H, NO₂; R₂ = aminomethyl) were obtained by aminomethylating II (R₂ = H). II (X = O, R₁ = NH₂, R₂ = H) was treated with MeCOCH₂CO₂Et to give II (X = O, R₁ = NHCOCH₂CO₂Me, R₂ = H) which was treated with 4-R₃C₆H₄N₂⁺ (R₃ = H, Me, OMe) to give II [X = O, R₁ = 4-R₃C₆H₄N:NC(:CMeOH)CONH, R₂ = H].

10/ 562,112

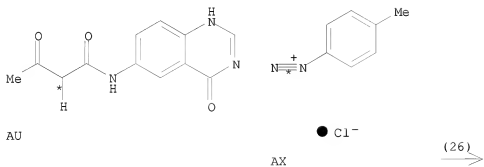
RX(25) OF 32 ...AU + AV ==> AW



AW

RX(25) RCT AU 40368-25-0, AV 100-34-5
PRO AW 345627-06-7

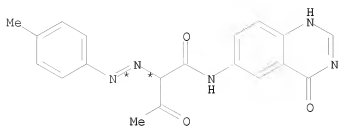
RX(26) OF 32 ...AU + AX ==> AY



AU

AX

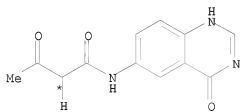
(26)



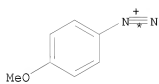
AY

RX(26) RCT AU 40368-25-0, AX 2028-84-4
PRO AY 82436-16-6

RX(27) OF 32 ...AU + AZ ==> BA

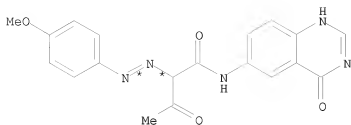


AU



AZ

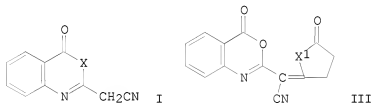




BA

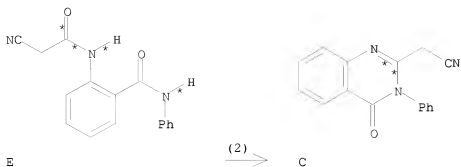
RX(27) RCT AU 40368-25-0, AZ 4346-59-2
PRO BA 82436-17-7

L3 ANSWER 213 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 96:20043 CASREACT
TITLE: Reactions of 2-cyanomethyl-3,1-benzoxazin-4(H)-one
with nucleophilic reagents, acid anhydrides and acid
imides
AUTHOR(S): Mohamed, M. M.; El-Hashash, M. A.; Esswy, A.; Shaban,
M. E.
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
SOURCE: Indian Journal of Chemistry, Section B: Organic
Chemistry Including Medicinal Chemistry (1981),
20B(8), 718-19
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



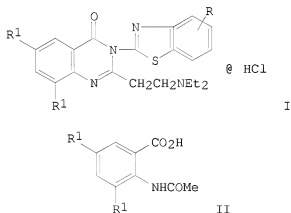
AB Refluxing benzoxazinone (I) (X = O) (II) with N₂H₄ and PhNHNH₂ in EtOH
gave I (X = NNH₂, NNHPh), resp., whereas refluxing II with PhNH₂ in EtOH
gave 2-PhNHCOC₆H₄NHCOCH₂CN. Condensation of II with succinic anhydride
and succinimide gave III (X₁ = O, NH), resp.

RX(2) OF 22 ...E ==> C



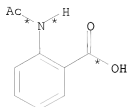
RX(2) RCT E 79946-29-5
 PRO C 20873-23-8
 CAT 108-24-7 Ac2O

L3 ANSWER 214 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 96:6681 CASREACT
 TITLE: Synthesis of some new 4(3H)-quinazolinones as
 potential fungicides
 AUTHOR(S): Chaurasia, M. R.; Sharma, Surendra K.; Kumar, Sunil
 CORPORATE SOURCE: Dep. Chem., D.A.V. Coll., Dehra Dun, 248 001, India
 SOURCE: Current Science (1981), 50(19), 841-3
 CODEN: CUSCAM; ISSN: 0011-3891
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

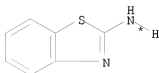


AB Benzothiazolylquinazolines I (R = H, 4-, 5-, 6-Me, 4-, 5-, 6-Cl, 6-MeO, 6-EtO, R1 = H, Br) were prepared in 32-71% yields by cyclocondensation of II in the presence of an appropriate 2-aminobenzimidazole to give intermediates (no data) which were condensed with CH2O and Et2NH.HCl. I inhibited *Aspergillus niger* and *Draschlera australiensis*.

RX(1) OF 3 A + B ==> C...

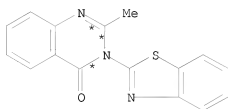


A



B

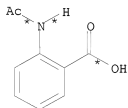
(1) →



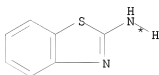
C

RX(1) RCT A 89-52-1, B 136-95-8
 PRO C 81762-52-9

RX(3) OF 3 COMPOSED OF RX(1), RX(2)
 RX(3) A + B + D + E ==> F



A



B

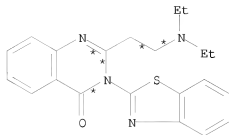


D



E

2
STEPS
→



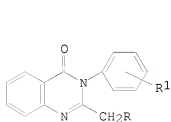
● HCl

F

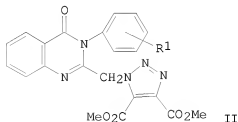
RX(1) RCT A 89-52-1, B 136-95-8
PRO C 81762-52-9

RX(2) RCT C 81762-52-9, D 109-89-7, E 50-00-0
PRO F 80144-66-7

L3 ANSWER 215 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 96,6679 CASREACT
TITLE: Quinazolinones. 2. Syntheses and some reactions of
2-azidomethyl-3-aryl-4-quinazolinones
AUTHOR(S): Domanig, Rainer
CORPORATE SOURCE: Inst. Org. Pharm. Chem., Univ. Innsbruck, Innsbruck,
A-6020, Austria
SOURCE: Monatshefte fuer Chemie (1981), 112(10), 1195-202
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I

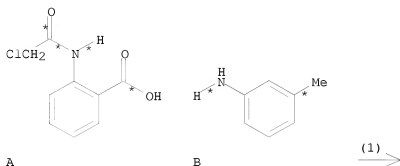


II

AB Starting with the chloromethyl compds. I (R = Cl; R1 = H, 2-Me, 2-MeO, 2-NO2, 3-MeO, 3,5-(MeO)2, 4-Cl, 5-NO2), the new 2-azidomethyl-3-aryl-4-quinazolinones I (R = N3) were prepared, some of which were reduced to the corresponding amines I (R = NH2) by H2S in good

yield. As a first example of the capability of the azides to undergo 1,3-dipolar cycloaddn., II (R1 = 2-Me, 3-MeO, 4-Cl) were prepared by reacting I (R = N3) with MeO2CC.tplbond.CC(=O)OMe.

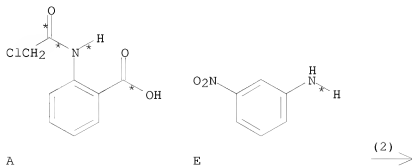
RX(1) OF 16 A + B ==> C



C

RX(1) RCT A 14422-49-2, B 108-44-1
 PRO C 76535-03-0
 SOL 108-88-3 PhMe

RX(2) OF 16 A + E ==> F

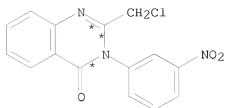


A

E

(2) →

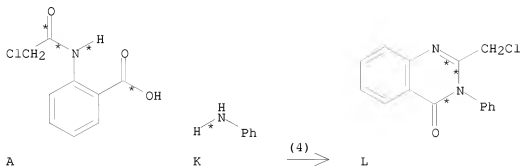
10/ 562,112



F

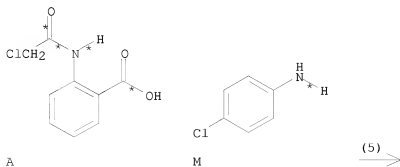
RX(2) RCT A 14422-49-2, E 99-09-2
 PRO F 80096-24-8
 SOL 108-88-3 PhMe

RX(4) OF 16 A + K ==> L

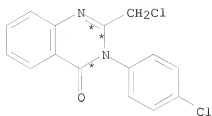


RX(4) RCT A 14422-49-2, K 62-53-3
 PRO L 22312-77-2
 SOL 108-88-3 PhMe

RX(5) OF 16 A + M ==> N



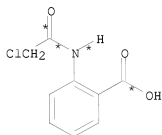
10/ 562,112



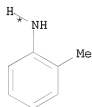
N

RX(5) RCT A 14422-49-2, M 106-47-8
 PRO N 22280-87-1
 SOL 108-88-3 PhMe

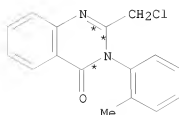
RX(6) OF 16 A + O ==> P



A



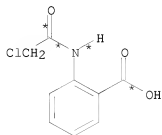
O



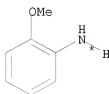
P

RX(6) RCT A 14422-49-2, O 95-53-4
 PRO P 3166-54-9
 SOL 108-88-3 PhMe

RX(8) OF 16 A + S ==> T



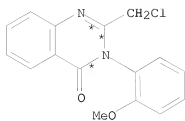
A



S



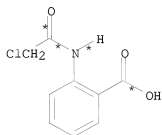
10/ 562,112



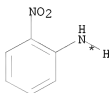
T

RX(8) RCT A 14422-49-2, S 90-04-0
 PRO T 22312-81-8
 SOL 108-88-3 PhMe

RX(9) OF 16 A + U ==> V

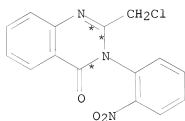


A



U

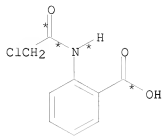
(9) →



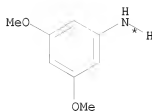
V

RX(9) RCT A 14422-49-2, U 88-74-4
 PRO V 80096-22-6
 SOL 108-88-3 PhMe

RX(10) OF 16 A + W ==> X

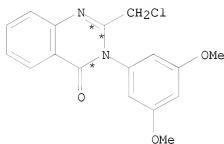


A



W

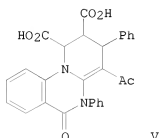
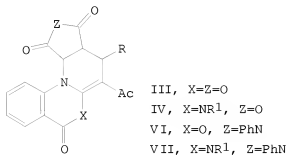
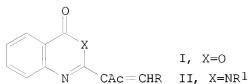
(10) →



X

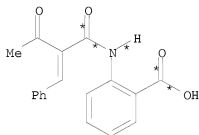
RX(10) RCT A 14422-49-2, W 10272-07-8
 PRO X 80096-23-7
 SOL 108-88-3 PhMe

L3 ANSWER 216 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 95:115443 CASREACT
 TITLE: Synthesis and reactions of
 2-(α -acetylstyryl)-3,1-benzoxazin-(4H)-ones and
 2-(α -acetylstyryl)-quinazolin-4-(3H)-ones
 Elkasaby, M. A.; Nouredin, N. A.
 AUTHOR(S): Fac. Sci., Ain Shams Univ., Cairo, Egypt
 CORPORATE SOURCE: Indian Journal of Chemistry, Section B: Organic
 SOURCE: Chemistry Including Medicinal Chemistry (1981),
 20B(4), 290-3
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

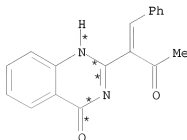


AB Benzoxazinones I (R = Ph, p-MeOC₆H₄, p-Me₂NC₆H₄) and quinazolines II (R = Ph, p-MeOC₆H₄; R¹ = H, Ph, p-MeC₆H₄, p-MeOC₆H₄) were prepared from o-HO₂CC₆H₄NHCOAc:CHR. I (R = Ph, p-MeOC₆H₄) react with maleic anhydride to give furopyridobenzoxazines III. Several II similarly underwent Diels-Alder reaction with maleic anhydride to give the furopyridoquinazolines IV. IV (R = R¹ = Ph) was hydrolyzed to give the pyridoquinazolinone V. II and III reacted with N-phenylmaleimide to give cycloadducts VI and VII, resp. Reaction of I with Grignard reagent and II with PhSH were investigated.

RX(35) OF 102 COMPOSED OF RX(1), RX(7)
RX(35) A ==> L



2
STEPS
→



A

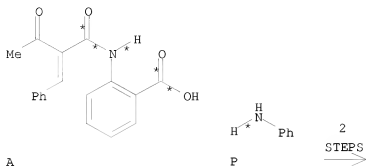
L

RX(1) RCT A 78817-80-8
PRO B 70723-60-3
CAT 108-24-7 Ac2O

RX(7) RCT B 70723-60-3
RGT M 7664-41-7 NH₃
PRO L 78817-49-9

10/ 562,112

RX(36) OF 102 COMPOSED OF RX(1), RX(10)
 RX(36) A + P ==> Q

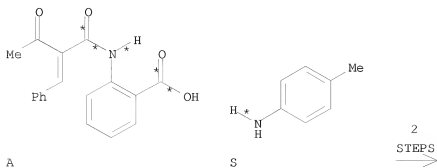


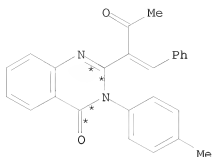
Q

RX(1) RCT A 78817-80-8
 PRO B 70723-60-3
 CAT 108-24-7 Ac2O

RX(10) RCT B 70723-60-3, P 62-53-3
 PRO Q 344572-47-0

RX(37) OF 102 COMPOSED OF RX(1), RX(12)
 RX(37) A + S ==> T



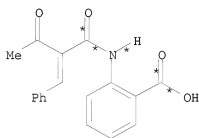


T

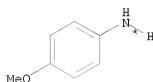
RX(1) RCT A 78817-80-8
 PRO B 70723-60-3
 CAT 108-24-7 Ac2O

RX(12) RCT B 70723-60-3, S 106-49-0
 PRO T 344571-95-5

RX(38) OF 102 COMPOSED OF RX(1), RX(14)
 RX(38) A + V ==> W

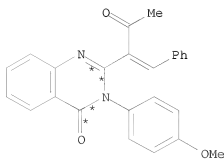


A



V

2
 STEPS
 →



W

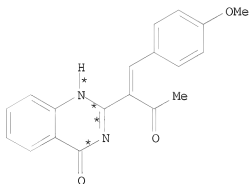
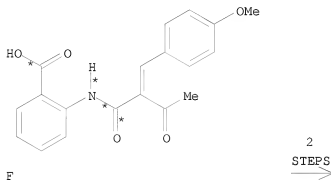
10/ 562,112

RX(1) RCT A 78817-80-8
PRO B 70723-60-3
CAT 108-24-7 Ac2O

RX(14) RCT B 70723-60-3, V 104-94-9
PRO W 344580-68-3

RX(49) OF 102 COMPOSED OF RX(3), RX(8)

RX(49) F ==> N

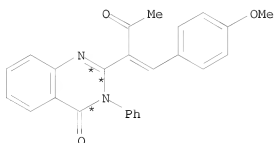
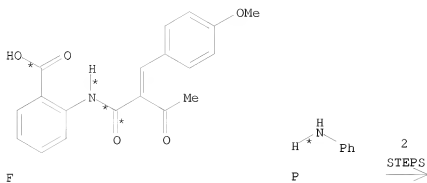


RX(3) RCT F 78817-81-9
PRO G 70723-63-6
CAT 108-24-7 Ac2O

RX(8) RCT G 70723-63-6
RGT M 7664-41-7 NH3
PRO N 78817-50-2

RX(50) OF 102 COMPOSED OF RX(3), RX(11)

RX(50) F + F ==> R



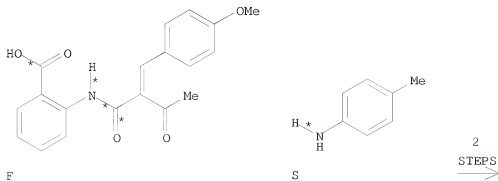
R

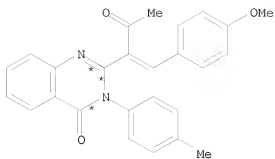
RX(3) RCT F 78817-81-9
 PRO G 70723-63-6
 CAT 108-24-7 Ac20

RX(11) RCT G 70723-63-6, P 62-53-3
 PRO R 344580-63-8

RX(51) OF 102 COMPOSED OF RX(3), RX(13)

RX(51) F + S ==> U



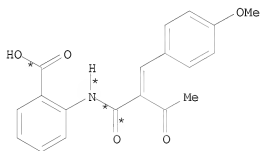


U

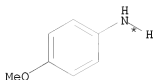
RX(3) RCT F 78817-81-9
 PRO G 70723-63-6
 CAT 108-24-7 Ac2O

RX(13) RCT G 70723-63-6, S 106-49-0
 PRO U 344581-72-2

RX(52) OF 102 COMPOSED OF RX(3), RX(15)
 RX(52) F + V ==> X

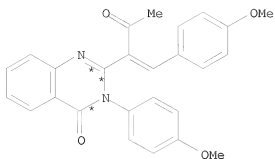


F



V

2
 STEPS
 →

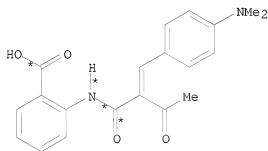


X

RX(3) RCT F 78817-81-9
 PRO G 70723-63-6
 CAT 108-24-7 Ac2O

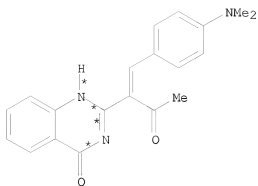
RX(15) RCT G 70723-63-6, V 104-94-9
 PRO X 344586-86-3

RX(59) OF 102 COMPOSED OF RX(5), RX(9)
 RX(59) I ==> O



I

2
 STEPS
 →

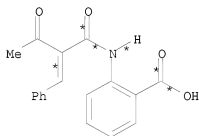


O

RX(5) RCT I 78817-82-0
 PRO J 78817-48-8
 CAT 108-24-7 Ac2O

RX(9) RCT J 78817-48-8
 RGT M 7664-41-7 NH3
 PRO O 78922-69-7

RX(77) OF 102 COMPOSED OF RX(1), RX(7), RX(31)
 RX(77) A + AT ==> AU

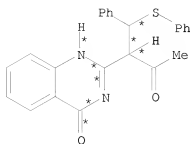


A



AT

3
 STEPS
 →



AU

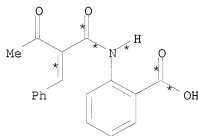
YIELD 70%

RX(1) RCT A 78817-80-8
 PRO B 70723-60-3
 CAT 108-24-7 Ac2O

RX(7) RCT B 70723-60-3
 RGT M 7664-41-7 NH3
 PRO L 78817-49-9

RX(31) RCT L 78817-49-9, AT 108-98-5
 PRO AU 78817-76-2

RX(81) OF 102 COMPOSED OF RX(1), RX(10), RX(32)
 RX(81) A + P + AT ==> AV



A



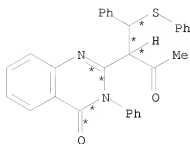
P



AT

3
 STEPS
 →

10/ 562,112



AV

YIELD 70%

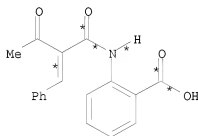
RX(1) RCT A 78817-80-8
PRO B 70723-60-3
CAT 108-24-7 Ac2O

RX(10) RCT B 70723-60-3, P 62-53-3
PRO Q 344572-47-0

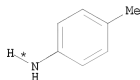
RX(32) RCT Q 344572-47-0, AT 108-98-5
PRO AV 78817-77-3

RX(84) OF 102 COMPOSED OF RX(1), RX(12), RX(33)

RX(84) A + S + AT ==> AW



A

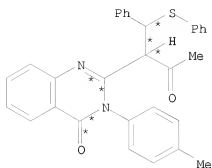


S



AT

3
STEPS
→



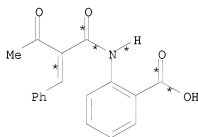
AW
YIELD 70%

RX(1) RCT A 78817-80-8
PRO B 70723-60-3
CAT 108-24-7 Ac2O

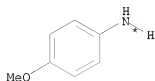
RX(12) RCT B 70723-60-3, S 106-49-0
PRO T 344571-95-5

RX(33) RCT T 344571-95-5, AT 108-98-5
PRO AW 78817-78-4

RX(87) OF 102 COMPOSED OF RX(1), RX(14), RX(34)
RX(87) A + V + AT ==> AX



A

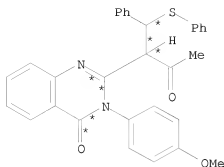


V



AT

3
STEPS
→



AX

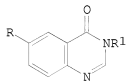
YIELD 70%

RX(1) RCT A 78817-80-8
 PRO B 70723-60-3
 CAT 108-24-7 Ac2O

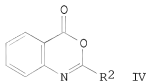
RX(14) RCT B 70723-60-3, V 104-94-9
 PRO W 344580-68-3

RX(34) RCT W 344580-68-3, AT 108-98-5
 PRO AX 78817-79-5

L3 ANSWER 217 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 95:115442 CASREACT
 TITLE: Reactions of some 4(3H)quinazolinones
 AUTHOR(S): Anwar, M.
 CORPORATE SOURCE: Fac. Sci., Tanta Univ., Tanta, Egypt
 SOURCE: Revue Roumaine de Chimie (1981), 26(4), 639-45
 CODEN: RRCHAX; ISSN: 0035-3930
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



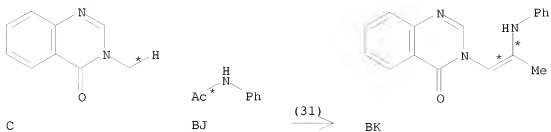
I



IV

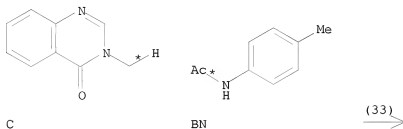
AB The reaction of I (R = H, NO₂; R₁ = H) with halo compds. gave I (R = H, R₁ = Me (II), Ac (III)); R = NO₂, R₁ = Me, Et, Ac, Bz, SO₂C₆H₄Me-4]. III and IV (R₂ = Ph, CH:CHC₆H₄OMe-4, CH:CHC₆H₄Cl-2) underwent aminolysis. II underwent fusion with aldehydes, ketones, benzil, and anilides. II condensed with maleic, succinic, and phthalic anhydrides. III underwent condensation with aldehydes.

RX(31) OF 86 ...C + BJ ==> BK



RX(31) RCT C 2436-66-0, BJ 103-84-4
 PRO BK 78875-23-7

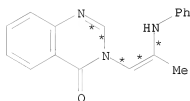
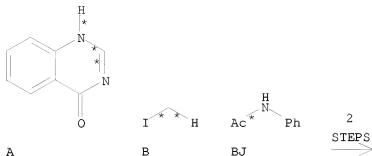
RX(33) OF 86 ...C + BN ==> BO



BO

RX(33) RCT C 2436-66-0, BN 103-89-9
 PRO BO 78875-25-9

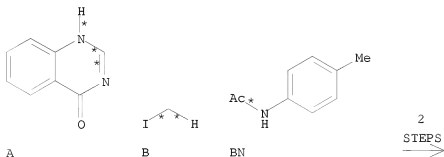
RX(62) OF 86 COMPOSED OF RX(1), RX(31)
 RX(62) A + B + BJ ==> BK

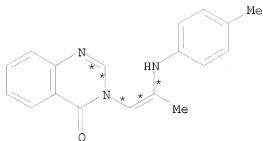


RX(1) RCT A 491-36-1, B 74-88-4
 PRO C 2436-66-0

RX(31) RCT C 2436-66-0, BJ 103-84-4
 PRO BK 78875-23-7

RX(64) OF 86 COMPOSED OF RX(1), RX(33)
 RX(64) A + B + BN ==> BO



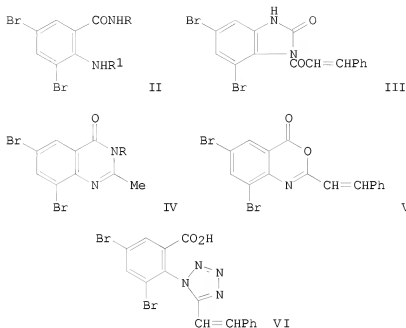


BO

RX(1) RCT A 491-36-1, B 74-88-4
PRO C 2436-66-0

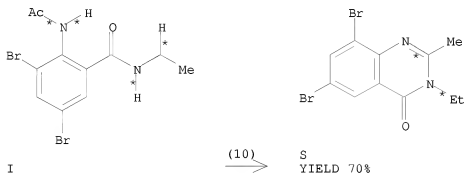
RX(33) RCT C 2436-66-0, BN 103-89-9
PRO BO 78875-25-9

L3 ANSWER 218 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 95:115418 CASREACT
 TITLE: Reaction of 6,8-dibromo-2-methyl-3,1-benzoxazin-4(H)-one with some nucleophilic reagents: synthesis of quinazoline, tetrazole and benzimidazole derivatives
 AUTHOR(S): Ismail, M. F.; Shams, N. A.; Naguib, M. I.
 CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1981), 20B(5), 394-7
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



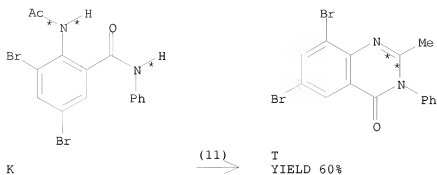
AB The reaction of 6,8-dibromo-2-methyl-3,1(4H)-benzoxazin-4-one (I) with RNH₂ (R = Et, Ph, NH₂, NHPH, OH, NHCONH₂) to give II (R₁ = Ac, PhCH:CH), and III. II (R₁ = Ac) cyclized to quinazolones IV. I condensed with PhCHO to give benzoxazine V, which was converted to II (R = CH₂Ph, Ph; R₁ = COCH:CHPh). V treated with HN₃ gave VI and III.

RX(10) OF 40 ...I ==> S...



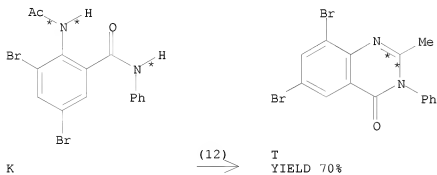
RX(10) RCT I 78993-23-4
PRO S 79008-15-4

RX(11) OF 40 ...K ==> T...



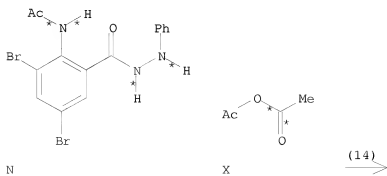
RX(11) RCT K 78993-24-5
RGT U 10025-87-3 POC13
PRO T 4145-21-5

RX(12) OF 40 K ==> T

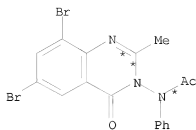


RX(12) RCT K 78993-24-5
PRO T 4145-21-5

RX(14) OF 40 ...N + X ==> Y



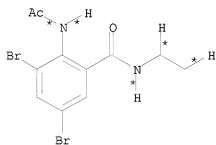
10/ 562,112



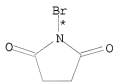
Y
YIELD 72%

RX(14) RCT N 78993-26-7, X 108-24-7
PRO Y 78993-29-0

RX(35) OF 40 COMPOSED OF RX(10), RX(15)
RX(35) I + Z ==> AA

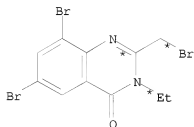


I



Z

2
STEPS
→



AA
YIELD 22%

RX(10) RCT I 78993-23-4
PRO S 79008-15-4

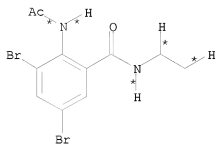
RX(15) RCT S 79008-15-4, Z 128-08-5

10/ 562,112

PRO AA 78993-36-9

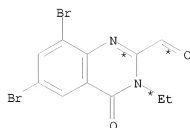
RX(36) OF 40 COMPOSED OF RX(10), RX(16)

RX(36) I ==> AB



I

2
STEPS
→



AB
YIELD 40%

RX(10) RCT I 78993-23-4

PRO S 79008-15-4

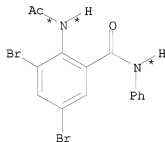
RX(16) RCT S 79008-15-4

RGT AC 7446-08-4 SeO2

PRO AB 78993-30-3

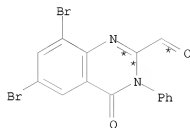
RX(37) OF 40 COMPOSED OF RX(11), RX(17)

RX(37) K ==> AD



K

2
STEPS
→



AD
YIELD 54%

RX(11) RCT K 78993-24-5

RGT U 10025-87-3 POC13

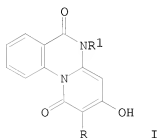
PRO T 4145-21-5

RX(17) RCT T 4145-21-5

RGT AC 7446-08-4 SeO2

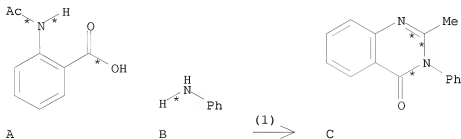
PRO AD 78993-31-4

L3 ANSWER 219 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 95:7205 CASREACT
 TITLE: A new route to 1H-pyrido[1,2-a]quinazolines
 AUTHOR(S): Soliman, Farid S. G.; Stadlbauer, Wolfgang; Kappe, Thomas
 CORPORATE SOURCE: Fac. Pharm., Univ. Alexandria, Alexandria, Egypt
 SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1981), 36B(2), 252-6
 CODEN: ZNBAD2; ISSN: 0340-5087
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



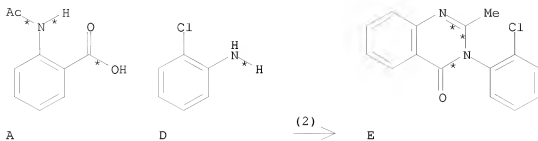
AB The pyridoquinazolinones I (R = PhCH₂, Et, Ph, Me₂CH, Bu, R₁ = Ph, p-BrC₆H₄, o-ClC₆H₄, o-MeC₆H₄) were prepared by reacting monosubstituted bis(2,4,6-trichlorophenyl) malonates with 3-aryl-3,4-dihydro-2-methyl-4-quinazolinones. Allylation of I (R = R₁ = Ph) with allyl bromide afforded the corresponding 3-allyloxy derivative. Certain generalizations of the cleavage processes of this series in the mass spectra are reported.

RX(1) OF 27 A + B ==> C...



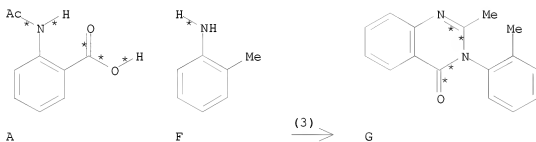
RX(1) RCT A 89-52-1, B 62-53-3
 PRO C 2385-23-1

RX(2) OF 27 A + D ==> E...



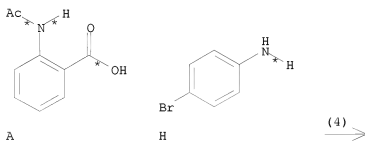
RX(2) RCT A 89-52-1, D 95-51-2
 PRO E 340-57-8

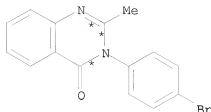
RX(3) OF 27 A + F \implies G...



RX(3) RCT A 89-52-1, F 95-53-4
 PRO G 72-44-6

RX(4) OF 27 A + H \implies I...

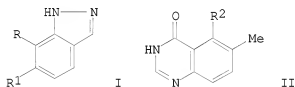




I
YIELD 44%

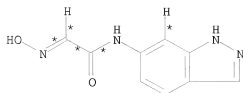
RX(4) RCT A 89-52-1, H 106-40-1
PRO I 1788-95-0

L3 ANSWER 220 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 95:7138 CASREACT
TITLE: Nucleosides. Part 40. Synthesis of a [3,4-f]-linked
pyrazoloquinazolinone
AUTHOR(S): Lichtenthaler, Frieder W.; Cuny, Eckehard
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Tech. Hochsch. Darmstadt,
Darmstadt, D-6100, Fed. Rep. Ger.
SOURCE: Heterocycles (1981), 15(2), 1053-9
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The pyrazoloquinazolinone I (RR1 = CONHCH:N) was prepared by 2 methods. Thus I (R = H, R1 = NH2) were treated with Cl3CCCHO and NH2OH to give I (R = H, R1 = NHCOCH:NOH) which was cyclized with acid and oxidized with H2O2 to give I (R = CO2H, R1 = NH2). Esterification of acid and cyclization with HCONH2 gave I (RR1 = CONHCH:N). Alternatively II (R2 = H) was nitrated and II (R2 = NO2) reduced to the amine, diazotized, and cyclized with Me2NOAc.

RX(25) OF 26 COMPOSED OF RX(3), RX(4), RX(5), RX(2)
RX(25) C + L + F ==> G

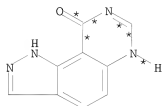


C

L

F

4
STEPS
→

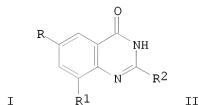
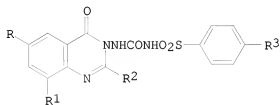


G

YIELD 74%

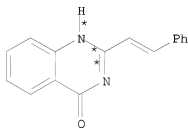
RX(3)	RCT	C 77929-34-1
	RGT	I 7664-93-9 H2SO4
	PRO	H 73907-94-5
RX(4)	RCT	H 73907-94-5
	RGT	K 7722-84-1 H2O2
	PRO	J 73907-95-6
RX(5)	RCT	J 73907-95-6, L 334-88-3
	PRO	E 73907-98-9
RX(2)	RCT	E 73907-98-9, F 75-12-7
	PRO	G 73907-90-1
	SOL	75-12-7 Formamide

arylsulfonylureas as hypoglycemic agents
 AUTHOR(S): Husain, M. Imtiaz; Srivastav, G. C.
 CORPORATE SOURCE: Dep. Chem., Lucknow Univ., Lucknow, 226 007, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (1980),
 19B(10), 916-17
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

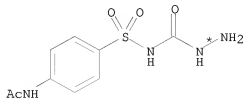


AB Thirty two new compds. I (R, R1 = H, Br; R2 = Ph, 2,3,5-HOBr2C6H2, CH:CHPh; R3 = H, Me, MeO, NHAc) were prepared by refluxing II with 4-R3C6H4SO2NHCONH2 in pyridine. I (R = H, R1 = Br, R2 = Ph, R3 = NHAc) showed 38% reduction in blood sugar level in rats at an oral dose of 250 mg/kg.

RX(25) OF 32 V + AF ==> AL

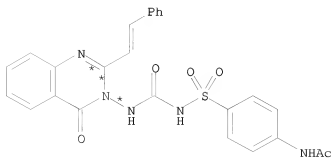


V



AF

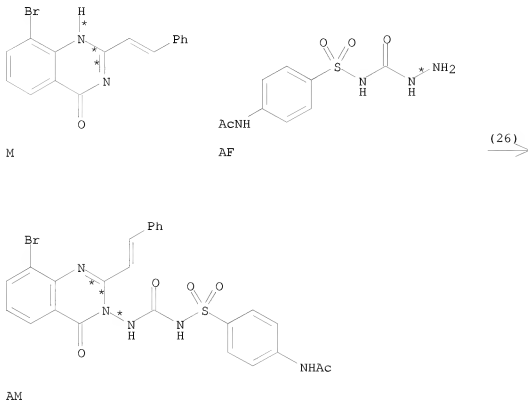
(25) →



AL

RX(25) RCT V 4765-58-6, AF 76983-56-7
 PRO AL 344595-28-4
 CAT 110-86-1 Pyridine

RX(26) OF 32 M + AF ==> AM

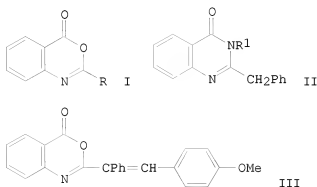


RX(26) RCT M 76983-54-5, AF 76983-56-7
 PRO AM 344608-04-4
 CAT 110-86-1 Pyridine

L3 ANSWER 222 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 94:139722 CASREACT
 TITLE: Some reactions with 2-benzyl-4H-3,1-benzoxazine-4-one, 6-bromo-2-methyl-4H-3,1-benzoxazin-4-one and 2-benzyl-3-phenyl-4 (3H)-quinazolinone
 AUTHOR(S): El Hashash, M. A.; Sayed, M. A.
 CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
 SOURCE: Egyptian Journal of Chemistry (1980), Volume Date 1978, 21(2), 115-31
 CODEN: EGJCA3; ISSN: 0367-0422
 DOCUMENT TYPE: Journal

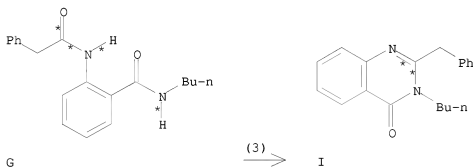
LANGUAGE:
GI

English



AB The benzoxazone I (R = PhCH₂) reacted with primary amines R₁NH₂ and gave o-R₁NHCOC₆H₄NHCOCH₂Ph (R₁ = Bu, PhCH₂, p-HO₂CC₆H₄) and the quinazolinones II (R₁ = p-HOC₆H₄, Ph). Aldehydes and acetophenone condensed with I (R = PhCH₂) and II (R₁ = Ph) and yielded styrylbenzoxazones, e.g. III and bisbenzoxazones. I (R = Ph) condensed with hydrazines, hydroxylamine and with active methylene compds. and yielded quinazolinones and a keto-ester, resp. Also, the reaction of I (R = Ph, Me) with aromatic hydrocarbons in presence of AlCl₃ and with aralkyl magnesium halides was described. P2S5 reacted with I (R = Me) and yielded the corresponding thione.

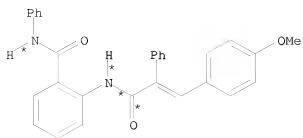
RX(3) OF 42 ...G ==> I



RX(3) RCT G 74772-51-3
 PRO I 74772-52-4
 CAT 108-24-7 Ac2O

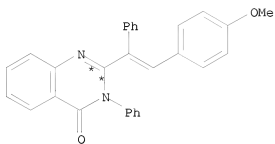
RX(10) OF 42 ...U ==> T

10/ 562,112



U

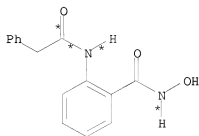
(10) \longrightarrow



T

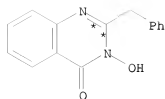
RX(10) RCT U 344610-95-3
 PRO T 344610-14-6
 CAT 108-24-7 Ac2O

RX(14) OF 42 Z ==> AA



Z

(14) \longrightarrow

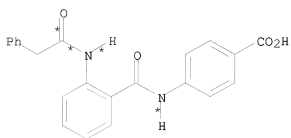


AA

RX(14) RCT Z 74772-63-7
 PRO AA 74772-62-6
 CAT 108-24-7 Ac2O

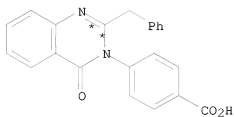
10/ 562,112

RX(17) OF 42 ...AF ==> AG



AF

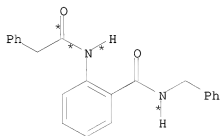
(17)



AG

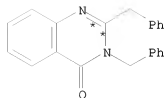
RX(17) RCT AF 76253-93-5
 PRO AG 76244-49-0
 CAT 108-24-7 Ac2O

RX(20) OF 42 ...AI ==> AL



AI

(20)

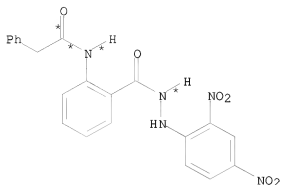


AL

RX(20) RCT AI 76253-92-4
 PRO AL 19857-42-2
 CAT 108-24-7 Ac2O

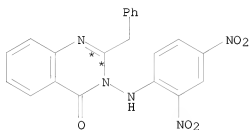
10/ 562,112

RX(24) OF 42 ...AR ==> AS



AR

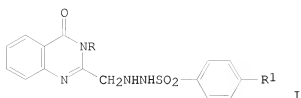
(24) →



AS

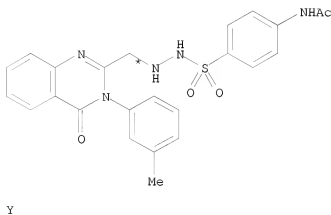
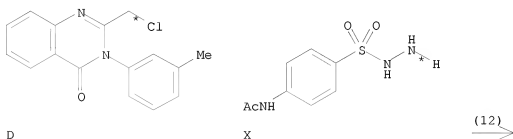
RX(24) RCT AR 76254-00-7
PRO AS 76253-99-1
CAT 108-24-7 Ac20

L3 ANSWER 223 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 94:84054 CASREACT
TITLE: Quinazolinone derivatives of etiological interest.
II. Synthesis and antibacterial activity of certain
3-aryl-2-(β-arylsulfonylhydrazinomethyl)-4(3H)-
quinazolinones
AUTHOR(S): Abdel-Aleem, A. M.; Abdel-Ghaffar, A. F.
CORPORATE SOURCE: Fac. Pharm. Microbiol., Assiut Univ., Assiut, Egypt
SOURCE: Indian Journal of Pharmaceutical Sciences (1980),
42(3), 79-81
CODEN: IJSIDW; ISSN: 0250-474X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



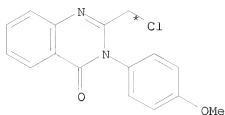
AB Quinazolinones I (R = 3-MeC6H4, 4-MeOC6H4, 4-ClC6H4, R1 = H, Me, NHAc, Br, Cl, NO2; R = Ph, 4-MeC6H4, 3-MeOC6H4, 4-BrC6H4, 3-ClC6H4, 4-EtO2CC6H4, 2-pyridyl, R1 = H) were prepared by treating the chloromethylquinazolinones with 4-R1C6H4SO2NHNH2. I had bactericidal activity less than that of sulfanilamide.

RX(12) OF 25 D + X ==> Y

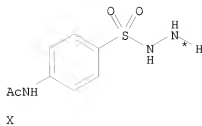


RX(12) RCT D 22312-79-4, X 3989-50-2
PRO Y 76534-89-9

RX(17) OF 25 J + X ==> AG

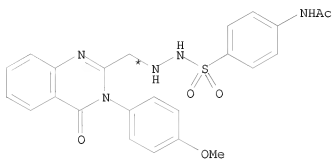


J



X

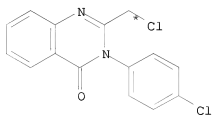
(17) \Rightarrow



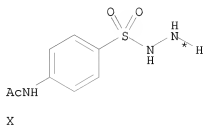
AG

RX(17) RCT J 22312-82-9, X 3989-50-2
PRO AG 76534-94-6

RX(22) OF 25 P + X \Rightarrow AL

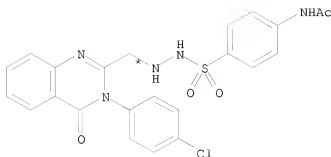


P



X

(22) \Rightarrow



AL

RX(22) RCT P 22280-87-1, X 3989-50-2
PRO AL 76534-99-1

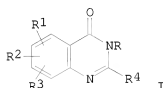
L3 ANSWER 224 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 94:15765 CASREACT
 TITLE: 4(3H)-Quinazolinones substituted with an aromatic group in the 3 position
 INVENTOR(S): Ishikawa, Masayuki; Tanaka, Hiromichi; Eguchi, Yukuo; Ito, Shigeru; Takashima, Yoshimi; Kobayashi, Masahiko
 PATENT ASSIGNEE(S): Japan
 SOURCE: Ger. Offen., 58 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2950376	A1	19800710	DE 1979-2950376	19791214
JP 55083761	A	19800624	JP 1978-155764	19781219
JP 56051461	A	19810509	JP 1979-126738	19791003
JP 56057768	A	19810520	JP 1979-133582	19791018
JP 56065877	A	19810603	JP 1979-141987	19791105
US 4276295	A	19810630	US 1979-103841	19791214
SE 7910376	A	19800620	SE 1979-10376	19791217
AU 7953932	A	19800626	AU 1979-53932	19791217
AU 526309	B2	19830106		
DK 7905399	A	19800620	DK 1979-5399	19791218
NO 7904135	A	19800620	NO 1979-4135	19791218
NL 7909118	A	19800623	NL 1979-9118	19791218
GB 2040927	A	19800903	GB 1979-43565	19791218
GB 2040927	B	19830126		
BE 880720	A1	19800619	BE 1979-198633	19791219
FR 2444671	A1	19800718	FR 1979-31059	19791219
FR 2444671	B1	19830610		
ZA 7906892	A	19801231	ZA 1979-6892	19791219
DD 150462	A5	19810902	DD 1979-217854	19791219
CA 1111849	A1	19811103	CA 1979-342295	19791219

HU 25076	A2	19830530	HU 1979-II311	19791219
HU 182733	B	19840328		
AT 7908011	A	19840115	AT 1979-8011	19791219
AT 375651	B	19840827		
CH 644112	A5	19840713	CH 1979-11257	19791219

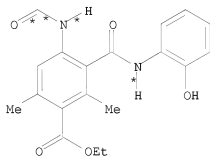
PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 94:15765
GI

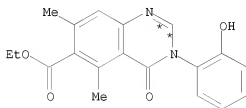


AB Quinazolinones I (R = optionally substituted Ph, pyridyl; R1, R3 = alkyl; R2 = alkoxy carbonyl; R4 = H, alkyl, halomethyl, CH₂OAc, CH₂OH) were prepared. Thus 2-amino-5-ethoxycarbonyl-4,6-dimethylbenzoic acid was treated with Ac₂O to give 95% 6-ethoxycarbonyl-2,5,7-trimethyl-3,1,4-benzoxazone, which was treated with 2-MeC₆H₄NH₂ to give 84.7% I (R = 2-MeC₆H₄, R1 = 5-Me, R2 = 6-CO₂Et, R3 = 7-Me, R4 = Me, II). At 3 + 10-5 M II gave 47 ± 6.4% relaxation of the thoracic artery in vitro.

RX(5) OF 10 J ==> K



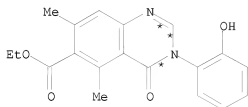
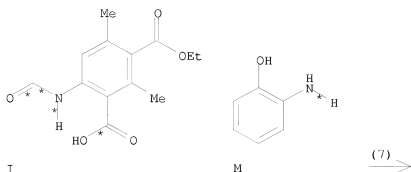
J



K

RX(5) RCT J 345584-73-8
PRO K 75913-00-7

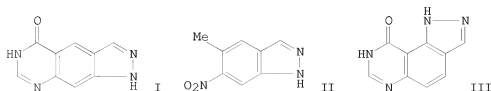
RX(7) OF 10 ...I + M ==> K



K

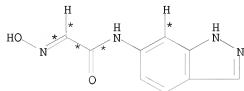
RX(7) RCT I 75913-88-1, M 95-55-6
 PRO K 75913-00-7

L3 ANSWER 225 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 94:3983 CASREACT
 TITLE: Nucleosides. 37. Benzologs of allopurinol: synthesis of pyrazolo[4,3-g] and [3,4-f]quinazolinones
 AUTHOR(S): Cuny, Eckehard; Lichtenthaler, F. W.; Moser, Alfred
 CORPORATE SOURCE: Inst. Org. Chem., Tech. Hochsch. Darmstadt, Darmstadt, D-6100, Fed. Rep. Ger.
 SOURCE: Tetrahedron Letters (1980), 21(32), 3029-32
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Pyrazoloquinazolinone I and its xanthine oxidase metabolite were prepared in 5 and 6 steps, resp., from indazole II, the key step being Niementowski type annulation of aminoindazolecarboxylic acids to give the pyrimidine ring. Two preps. of quinazolinone III by similar annulation, and by intramol. azo coupling (28% and 25% resp.) are reported.

RX(104) OF 120 COMPOSED OF RX(18), RX(19), RX(20), RX(4)
 RX(104) X + L + B ==> G



X

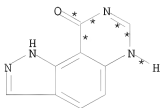


L



B

4
 STEPS
 →

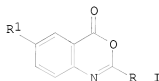


G
 YIELD 74%

RX(18)	RCT X 73907-93-4
	PRO Z 73907-94-5
RX(19)	RCT Z 73907-94-5
	PRO AA 73907-95-6
RX(20)	RCT AA 73907-95-6, L 334-88-3
	PRO F 73907-98-9
RX(4)	RCT F 73907-98-9, B 75-12-7
	PRO G 73907-90-1

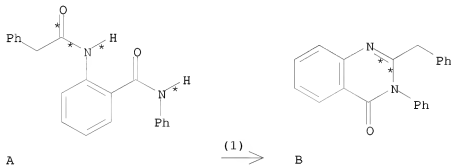
L3 ANSWER 226 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 93:114443 CASREACT
 TITLE: Synthesis of new sulfamoyl anilides.
 4H-3,1-benzoxazin-4-one and 4-quinazolinone derivatives
 of agricultural interest
 AUTHOR(S): El-Hashash, M. A.; Mohamed, M. M.; Sayed, M. A.
 CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt

SOURCE: Revue Roumaine de Chimie (1979), 24(11-12), 1509-20
 CODEN: RRCHAX; ISSN: 0035-3930
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Benzoxazinones I (R = CH₂Ph, R₁ = H; R = Me, R₁ = Br) reacted with sulfa compds., amines, aldehydes, hydrazines, NH₂OH, and active methylene compds. to give side chain-substituted benzoxazinones, quinazolones, and acylaminobenzoyl derivs. The products had herbicidal activity, but were generally ineffective as insecticides, fungicides, bactericides, and virucides.

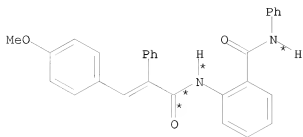
RX(1) OF 44 ...A ==> B...



RX(1) RCT A 74772-50-2
 PRO B 19857-34-2
 CAT 108-24-7 Ac2O

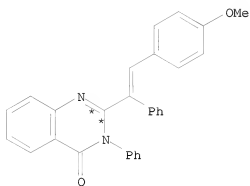
RX(20) OF 44 ...AL ==> AM

10/ 562,112



AL

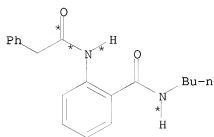
(20) \longrightarrow



AM

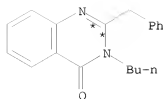
RX(20) RCT AL 74772-65-9
 PRO AM 74772-58-0
 CAT 108-24-7 Ac2O

RX(31) OF 44 ...AA ==> BB



AA

(31) \longrightarrow



BB

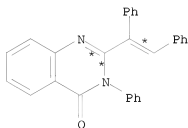
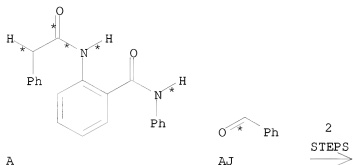
RX(31) RCT AA 74772-51-3
 PRO BB 74772-52-4

10/ 562,112

CAT 108-24-7 Ac2O

RX(35) OF 44 COMPOSED OF RX(1), RX(19)

RX(35) A + AJ ==> AK



AK

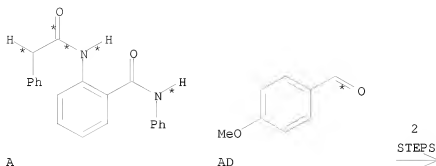
YIELD 65%

RX(1) RCT A 74772-50-2
PRO B 19857-34-2
CAT 108-24-7 Ac2O

RX(19) RCT B 19857-34-2, AJ 100-52-7
PRO AK 74772-57-9

RX(36) OF 44 COMPOSED OF RX(1), RX(32)

RX(36) A + AD ==> AM

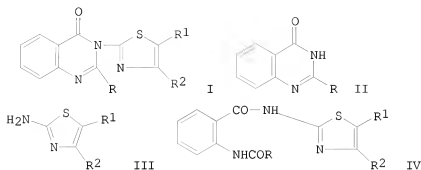


AM
YIELD 58%

RX(1) RCT A 74772-50-2
PRO B 19857-34-2
CAT 108-24-7 Ac2O

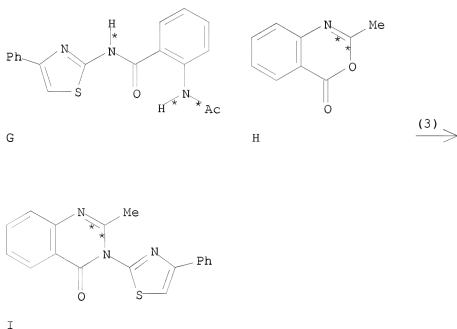
RX(32) RCT B 19857-34-2, AD 123-11-5
PRO AM 74772-58-0

L3 ANSWER 227 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 93:95222 CASREACT
TITLE: Synthesis of thiazolylquinazolin-4(3H)-ones
AUTHOR(S): Badr, M. Z. A.; El-Sherief, H. A. H.; El-Naggar, G. M.; Mahmoud, A. M.
CORPORATE SOURCE: Fac. Sci., Assiut Univ., Assiut, Egypt
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1979), 18B(6), 560-3
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB 3-Thiazolylquinazolin-4-ones I (R = Me, Ph; R1 = H, CO2Et; R2 = Ph, 4-MeC6H4, 4-MeOC6H4, 4-ClC6H4, 4-BrC6H4, Me) were prepared by condensing 3,1-benzoxazin-4(H)-ones II with aminothiazoles III. Heating 2-arylaminothiazoles IV in dry pyridine also give I. Heating 2-Styrylquinazolin-4-ones I (R = 4-O2NC6H4CH:CH, R1 = H, Ph, CO2Et, R2 = Ph, Me, 4-MeC6H4; R = 4-ClC6H4CH:CH, R1 = R2 = Ph) were prepared by condensing aromatic aldehydes with I (R = Me). I and IV showed bactericidal activity.

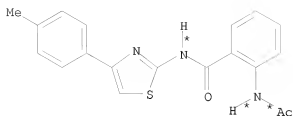
RX(3) OF 33 G + H ==> I...



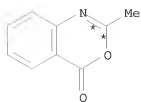
RX(3) RCT G 74636-72-9, H 525-76-8
 PRO I 74636-80-9

RX(5) OF 33 J + H ==> K...

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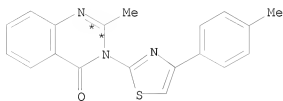


J



H

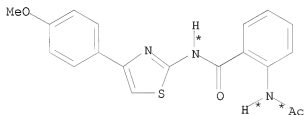
(5) \Rightarrow



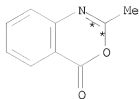
K

RX(5) RCT J 74636-73-0, H 525-76-8
PRO K 74636-85-4

RX(7) OF 33 M + H \Rightarrow N

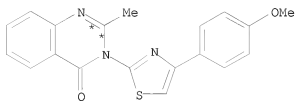


M



H

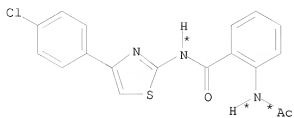
(7) \Rightarrow



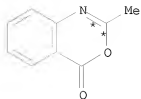
N

RX(7) RCT M 74636-74-1, H 525-76-8
PRO N 74636-81-0

RX(9) OF 33 P + H ==> Q

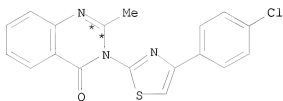


P



H

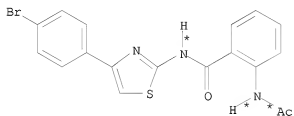
(9) ➞



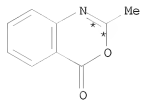
Q

 RX(9) RCT P 74636-75-2, H 525-76-8
 PRO Q 74636-82-1

RX(11) OF 33 S + H ==> T

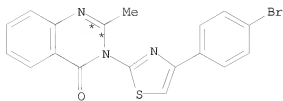


S



H

(11) ➞

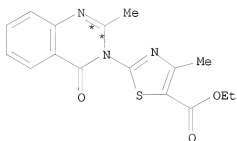
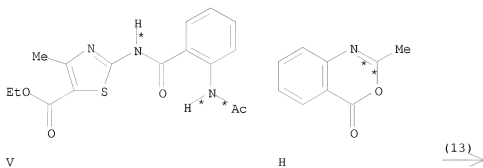


T

10/ 562,112

RX(11) RCT S 74636-76-3, H 525-76-8
PRO T 74636-83-2

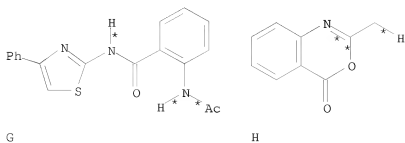
RX(13) OF 33 V + H ==> W...



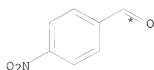
W

RX(13) RCT V 74636-77-4, H 525-76-8
PRO W 74636-84-3

RX(26) OF 33 COMPOSED OF RX(3), RX(22)
RX(26) G + H + AF ==> AH

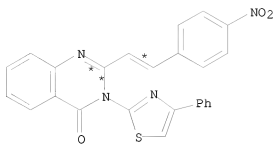


10/ 562,112



AF

2
STEPS
→

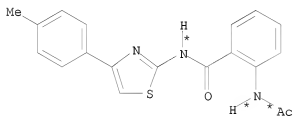


AH

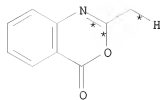
RX(3) RCT G 74636-72-9, H 525-76-8
PRO I 74636-80-9

RX(22) RCT I 74636-80-9, AF 555-16-8
PRO AH 74636-93-4

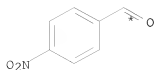
RX(28) OF 33 COMPOSED OF RX(5), RX(23)
RX(28) J + H + AF ==> AI



J

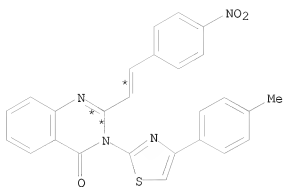


H



AF

2
STEPS
→

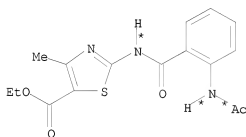


AI

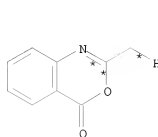
RX(5) RCT J 74636-73-0, H 525-76-8
PRO K 74636-85-4

RX(23) RCT K 74636-85-4, AF 555-16-8
PRO AI 74636-96-7

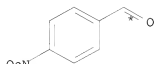
RX(30) OF 33 COMPOSED OF RX(13), RX(24)
RX(30) V + H + AF ==> AJ



V

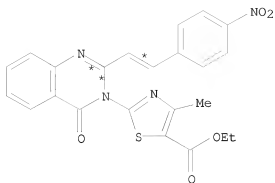


H



AF

2
STEPS
→



AJ

RX(13) RCT V 74636-77-4, H 525-76-8
PRO W 74636-84-3

RX(24) RCT W 74636-84-3, AF 555-16-8
PRO AJ 74636-94-5

L3 ANSWER 228 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 93:70766 CASREACT

TITLE: Acylantranils. 9. Influence of hydrogen bonding on the reaction of acetylanthranil with ammonia

AUTHOR(S): Errede, L. A.; Martinucci, P. D.; McBrady, J. J.

CORPORATE SOURCE: Res. Lab., 3M, St. Paul, MN, 55133, USA

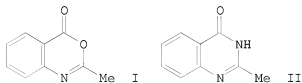
SOURCE: Journal of Organic Chemistry (1980), 45(15), 3009-17

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

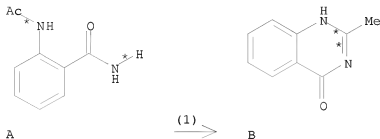
GI



AB H bonding has a marked influence on the reaction of acetylanthranil (I) with NH₃. The product of the reaction in anhydrous C₆H₆ is the quinazolinone II, but the rate of formation is unusually slow. The rate of this conversion is about 6 times faster in pyridine than in C₆H₆. If H₂O is added to the C₆H₆ system, the rate of reaction is increased by orders of magnitude, but the product is o-AcNHC₆H₄CONH₂ (III). In contrast, addition of H₂O to the pyridine system causes a small decrease in the rate and only a slight change in selectivity. These results are consistent with postulated mechanisms whereby I reacts with mol. clusters of NH₃, i.e.,

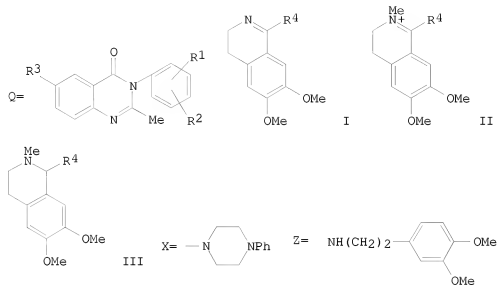
with $(\text{NH}_3)_n$ in C_6H_6 , with $\text{N}(\text{H}\cdot\text{S})_3$ in strong proton-acceptor solvents S , and with $(\text{NH}_3)_n\cdot\text{H}_2\text{O}$ in C_6H_6 containing added H_2O . III underwent cyclodehydration to give II.

RX(1) OF 4 ...A ==> B



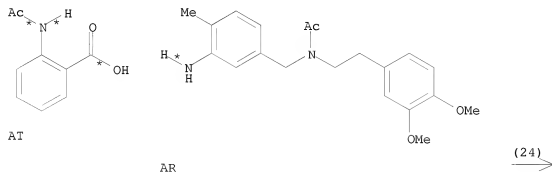
RX(1) RCT A 33809-77-7
PRO B 1769-24-0

L3 ANSWER 229 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 93:46560 CASREACT
 TITLE: Drugs acting on CNS: syntheses of
 2-methyl-3-o-tolylquinazolin-4-one (methaqualone)
 analogs
 AUTHOR(S): Prasad, Rajendra; Bhaduri, A. P.
 CORPORATE SOURCE: Div. Med. Chem., Cent. Drug Res. Inst., Lucknow,
 226001, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (1979),
 18B(5), 443-8
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

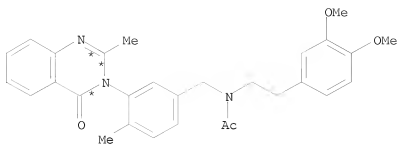


AB 3-Aryl-2-methyl-4(3H)-quinazolones [QH, QCO₂H, QC1 (R₁ = H, R₂ = 2-Cl, 3-Cl, 2-Me, 4-F; 4-Br; R₁ = R₂ = 3-Me; R₃ = iodo, H)] were prepared in 53-93% yields. Cyclization of QCONH(CH₂)₂C₆H₃(OMe)_{2-3,4} followed sequentially by iodomethylation of I [R₄ = Q (R₁ = 2-Me, R₂ = R₃ = H)] and NaBH₄ reduction of II [R₄ = Q (R₁ = 2-Me, R₂ = R₃ = H)] gave III [R₄ = Q (R₁ = 2-Me, R₂ = R₃ = H)]. Condensation of 2,5-Me(XCH₂)C₆H₃NH₂ and 2-AcNHC₆H₄CO₂H in the presence of dicyclohexylcarbodiimide gave QH (R₁ = 2-Me, R₂ = 5-XCH₂, R₃ = H). Also prepared was QH (R₁ = 2-Me, R₂ = CH₂Z, R₃ = H). None of the compds. possessed any central nervous system depressant activity. The LD₅₀ of the compds. was >1000 mg/kg i.p.

RX(24) OF 58 ...AT + AR ==> AU...



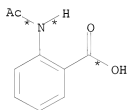
10/ 562,112



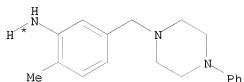
AU

RX(24) RCT AT 89-52-1, AR 74101-73-8
 PRO AU 74101-74-9
 CAT 538-75-0 DCC

RX(25) OF 58 ...AT + AQ ==> AW

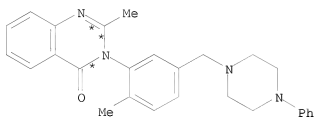


AT



AQ

(25) \longrightarrow

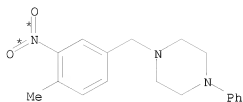


AW

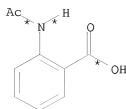
RX(25) RCT AT 89-52-1, AQ 74101-72-7
 PRO AW 74101-75-0
 CAT 538-75-0 DCC

RX(41) OF 58 COMPOSED OF RX(22), RX(25)

RX(41) AM + AT ==> AW

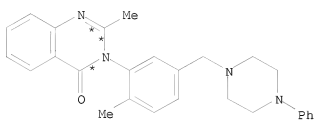


AM



AT

2
STEPS
→

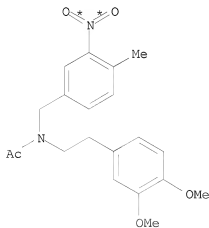


AW

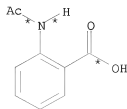
RX(22) RCT AM 74101-69-2
PRO AQ 74101-72-7

RX(25) RCT AT 89-52-1, AQ 74101-72-7
PRO AW 74101-75-0
CAT 538-75-0 DCC

RX(42) OF 58 COMPOSED OF RX(23), RX(24)
RX(42) AP + AT ==> AU

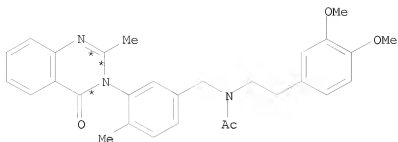


AP



AT

2
STEPS
→

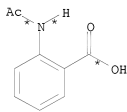


AU

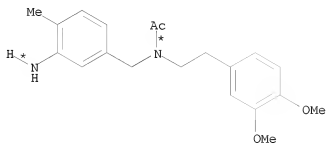
RX(23) RCT AP 74101-71-6
 PRO AR 74101-73-8
 SOL 64-17-5 EtOH

RX(24) RCT AT 89-52-1, AR 74101-73-8
 PRO AU 74101-74-9
 CAT 538-75-0 DCC

RX(43) OF 58 COMPOSED OF RX(24), RX(27)
 RX(43) AT + AR ==> AY



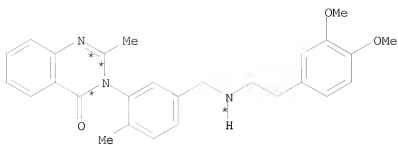
AT



AR

2
 STEPS
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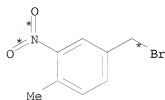
AY

YIELD 16%

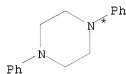
RX(24) RCT AT 89-52-1, AR 74101-73-8
 PRO AU 74101-74-9
 CAT 538-75-0 DCC

RX(27) RCT AU 74101-74-9
 RGT AZ 7647-01-0 HCl
 PRO AY 74101-76-1

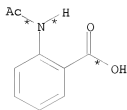
RX(48) OF 58 COMPOSED OF RX(19), RX(22), RX(25)
 RX(48) AJ + AL + AT ==> AW



AJ

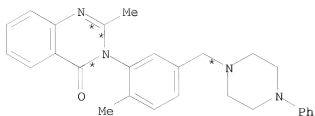


AL



AT

3
 STEPS
 ==>



AW

10/ 562,112

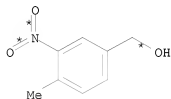
RX(19) RCT AJ 74101-68-1, AL 613-39-8
PRO AM 74101-69-2

RX(22) RCT AM 74101-69-2
PRO AQ 74101-72-7

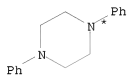
RX(25) RCT AT 89-52-1, AQ 74101-72-7
PRO AW 74101-75-0
CAT 538-75-0 DCC

RX(49) OF 58 COMPOSED OF RX(18), RX(19), RX(22), RX(25)

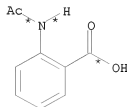
RX(49) AI + AL + AT ==> AW



AI

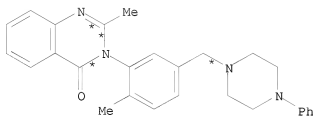


AL



AT

4
STEPS
→



AW

RX(18) RCT AI 40870-59-5
RGT AK 7789-60-8 PBr3
PRO AJ 74101-68-1

RX(19) RCT AJ 74101-68-1, AL 613-39-8
PRO AM 74101-69-2

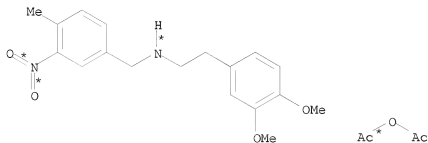
RX(22) RCT AM 74101-69-2
PRO AQ 74101-72-7

RX(25) RCT AT 89-52-1, AQ 74101-72-7

10/ 562,112

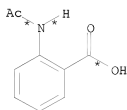
PRO AW 74101-75-0
CAT 538-75-0 DCC

RX(52) OF 58 COMPOSED OF RX(21), RX(23), RX(24)
RX(52) AO + I + AT ==> AU



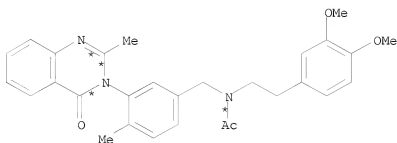
AO

I



AT

3
STEPS
→



AU

RX(21) RCT AO 74101-70-5, I 108-24-7
PRO AP 74101-71-6

RX(23) RCT AP 74101-71-6
PRO AR 74101-73-8
SOL 64-17-5 EtOH

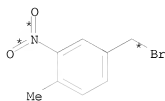
RX(24) RCT AT 89-52-1, AR 74101-73-8
PRO AU 74101-74-9

10/ 562,112

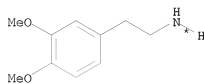
CAT 538-75-0 DCC

RX(53) OF 58 COMPOSED OF RX(20), RX(21), RX(23), RX(24)

RX(53) AJ + AN + I + AT ==> AU



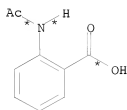
AJ



AN

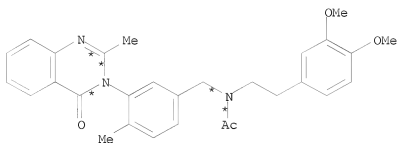


I



AT

4
STEPS
→



AU

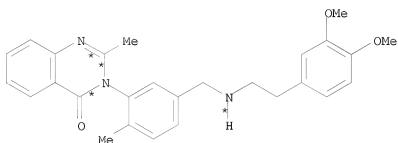
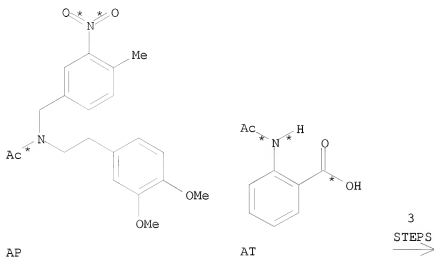
RX(20) RCT AJ 74101-68-1, AN 120-20-7
PRO AO 74101-70-5

RX(21) RCT AO 74101-70-5, I 108-24-7
PRO AP 74101-71-6

RX(23) RCT AP 74101-71-6
PRO AR 74101-73-8
SOL 64-17-5 EtOH

RX(24) RCT AT 89-52-1, AR 74101-73-8
PRO AU 74101-74-9
CAT 538-75-0 DCC

RX(54) OF 58 COMPOSED OF RX(23), RX(24), RX(27)
 RX(54) AP + AT ==> AY



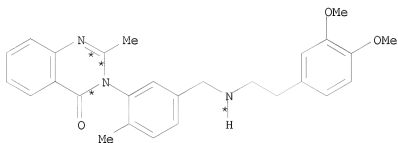
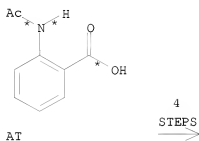
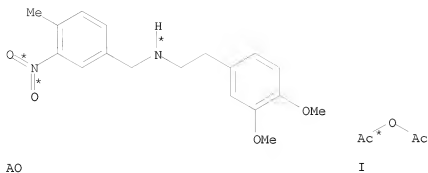
AY
 YIELD 16%

RX(23) RCT AP 74101-71-6
 PRO AR 74101-73-8
 SOL 64-17-5 EtOH

RX(24) RCT AT 89-52-1, AR 74101-73-8
 PRO AU 74101-74-9
 CAT 538-75-0 DCC

RX(27) RCT AU 74101-74-9
 RGT AZ 7647-01-0 HCl
 PRO AY 74101-76-1

RX(55) OF 58 COMPOSED OF RX(21), RX(23), RX(24), RX(27)
 RX(55) AO + I + AT ==> AY



YIELD 16%

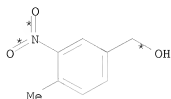
RX(21) RCT AO 74101-70-5, I 108-24-7
PRO AP 74101-71-6

RX(23) RCT AP 74101-71-6
PRO AR 74101-73-8
SOL 64-17-5 EtOH

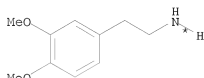
RX(24) RCT AT 89-52-1, AR 74101-73-8
PRO AU 74101-74-9
CAT 538-75-0 DCC

RX(27) RCT AU 74101-74-9
RGT AZ 7647-01-0 HCl
PRO AY 74101-76-1

RX(56) OF 58 COMPOSED OF RX(18), RX(20), RX(21), RX(23), RX(24)
 RX(56) AI + AN + I + AT ==> AU



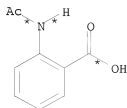
AI



AN

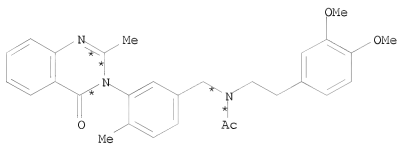


I



AT

5
 STEPS
 ➞



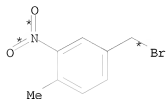
AU

RX(18)	RCT	AI 40870-59-5
	RGT	AK 7789-60-8 PBr3
	PRO	AJ 74101-68-1
RX(20)	RCT	AJ 74101-68-1, AN 120-20-7
	PRO	AO 74101-70-5
RX(21)	RCT	AO 74101-70-5, I 108-24-7
	PRO	AP 74101-71-6
RX(23)	RCT	AP 74101-71-6
	PRO	AR 74101-73-8
	SOL	64-17-5 EtOH

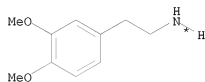
10/ 562,112

RX(24) RCT AT 89-52-1, AR 74101-73-8
 PRO AU 74101-74-9
 CAT 538-75-0 DCC

RX(57) OF 58 COMPOSED OF RX(20), RX(21), RX(23), RX(24), RX(27)
 RX(57) AJ + AN + I + AT ==> AY



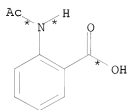
AJ



AN

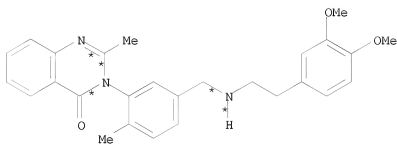


I



AT

5
 STEPS
 →



AY

YIELD 16%

RX(20) RCT AJ 74101-68-1, AN 120-20-7
 PRO AO 74101-70-5

RX(21) RCT AO 74101-70-5, I 108-24-7
 PRO AP 74101-71-6

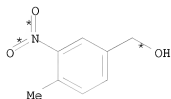
RX(23) RCT AP 74101-71-6
 PRO AR 74101-73-8
 SOL 64-17-5 EtOH

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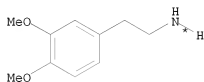
RX(24) RCT AT 89-52-1, AR 74101-73-8
PRO AU 74101-74-9
CAT 538-75-0 DCC

RX(27) RCT AU 74101-74-9
RGT AZ 7647-01-0 HCl
PRO AY 74101-76-1

RX(58) OF 58 COMPOSED OF RX(18), RX(20), RX(21), RX(23), RX(24), RX(27)
RX(58) AI + AN + I + AT ==> AY



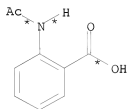
AI



AN

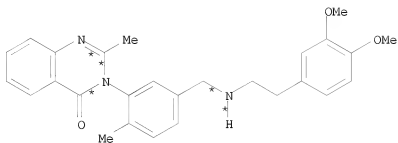


I



AT

6
STEPS
=>



AY
YIELD 16%

RX(18) RCT AI 40870-59-5
RGT AK 7789-60-8 PBr3
PRO AJ 74101-68-1

RX(20) RCT AJ 74101-68-1, AN 120-20-7
PRO AO 74101-70-5

RX(21) RCT AO 74101-70-5, I 108-24-7
 PRO AP 74101-71-6

RX(23) RCT AP 74101-71-6
 PRO AR 74101-73-8
 SOL 64-17-5 EtOH

RX(24) RCT AT 89-52-1, AR 74101-73-8
 PRO AU 74101-74-9
 CAT 538-75-0 DCC

RX(27) RCT AU 74101-74-9
 RGT AZ 7647-01-0 HCl
 PRO AY 74101-76-1

L3 ANSWER 230 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 93:26374 CASREACT

TITLE: Studies on biologically active halogenated compounds.
 II. Chemical modifications of
 6-amino-2-fluoromethyl-3-[o-tolyl]-4[3H]-quinazolinone

AUTHOR(S): Tani, Junichi; Yamada, Yoshihisa; Ochiai, Takashi;
 Ishida, Ryuichi; Inoue, Ichizo; Oine, Toyonari
 CORPORATE SOURCE: Res. Lab., Tanabe Seiyaku Co., Ltd., Osaka, 532, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1979), 27(11),
 2675-87

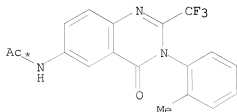
CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A number of derivs. of 6-amino-2-fluoromethyl-3-(o-tolyl)-4(3H)-quinazolinone (6-aminomethaqualone), a potent muscle relaxant, were prepared and screened in terms of the loss of righting reflex test and the rotating rod test in mice. Several derivs. with addnl. F substitution or with repositioning of the F atom exhibited high activities. Other structural modification included acylation, carbamoylation, and alkoxycarbonylation of the 6-amino group, hydroxylation at the 3-tolyl group, and replacement of the F atom at the 2-fluoromethyl group by O, N and S nucleophiles; these modification all resulted in loss of activity.

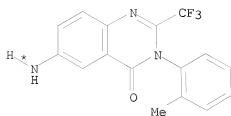
RX(2) OF 91 ...D ==> E



D

(2) →

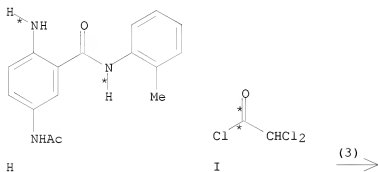
10/ 562,112



E

RX(2) RCT D 73832-50-5
 RGT F 7647-01-0 HCl
 PRO E 73832-08-3
 SOL 67-56-1 MeOH

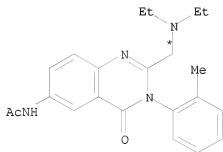
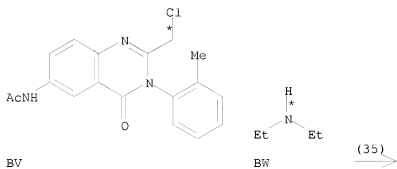
RX(3) OF 91 H + I ==> J



J

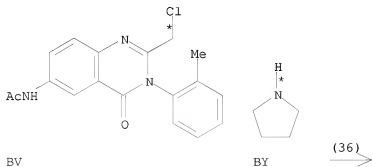
RX(3) RCT H 64102-81-4, I 79-36-7
 RGT K 7637-07-2 BF3
 PRO J 73832-51-6
 SOL 60-29-7 Et2O

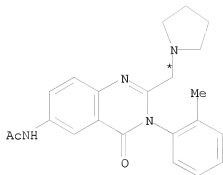
RX(35) OF 91 BV + BW ==> BX...



RX(35) RCT BV 61899-78-3, BW 109-89-7
 PRO BX 73832-71-0
 SOL 109-99-9 THF

RX(36) OF 91 BV + BY ==> BZ

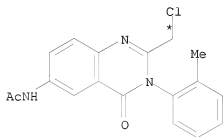




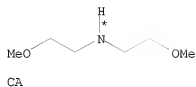
BZ

RX(36) RCT BV 61899-78-3, BY 123-75-1
 PRO BZ 73832-81-2
 SOL 109-99-9 THF

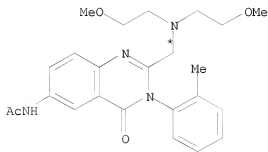
RX(37) OF 91 BV + CA ==> CB...



BV



(37)



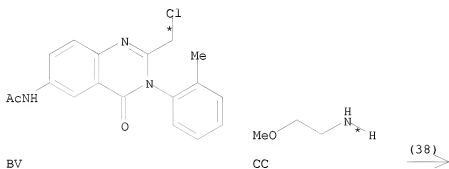
CB

RX(37) RCT BV 61899-78-3, CA 111-95-5
 PRO CB 73832-82-3

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SOL 109-99-9 THF

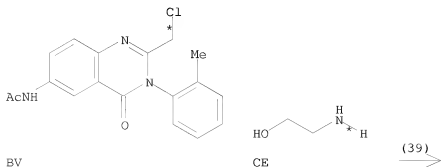
RX(38) OF 91 BV + CC ==> CD...

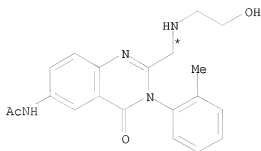


CD

RX(38) RCT BV 61899-78-3, CC 109-85-3
 PRO CD 73832-84-5
 SOL 109-99-9 THF

RX(39) OF 91 BV + CE ==> CF...

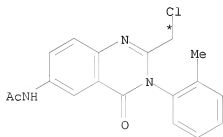




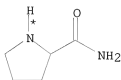
CF

RX(39) RCT BV 61899-78-3, CE 141-43-5
 PRO CF 73832-85-6
 SOL 109-99-9 THF

RX(40) OF 91 BV + CG ==> CH...

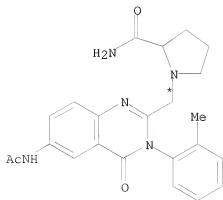


BV



CG

(40) →

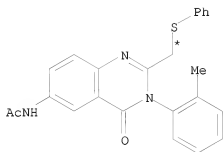
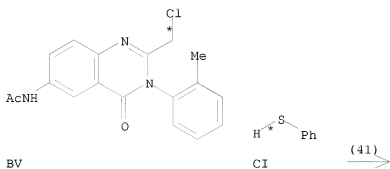


CH

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RX(40) RCT BV 61899-78-3, CG 2812-47-7
 PRO CH 73832-87-8
 SOL 109-99-9 THF

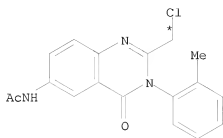
RX(41) OF 91 BV + CI ==> CJ...



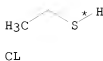
CJ

RX(41) RCT BV 61899-78-3, CI 108-98-5
 RGT CK 7646-69-7 NaH
 PRO CJ 73832-73-2
 SOL 109-99-9 THF

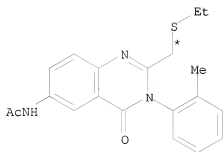
RX(42) OF 91 BV + CL ==> CM...



BV

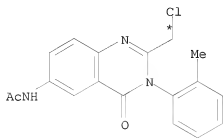


CL

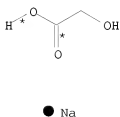
(42) \longrightarrow 

CM

RX(42) RCT BV 61899-78-3, CL 75-08-1
 RGT CK 7646-69-7 NaH
 PRO CM 73832-88-9
 SOL 109-99-9 THF

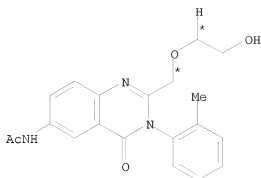
RX(43) OF 91 BV + CN \implies CO...

BV



CN

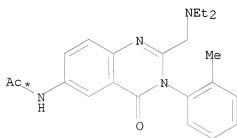
(43) \longrightarrow



CO

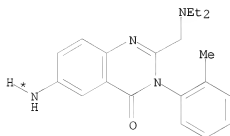
RX(43) RCT BV 61899-78-3, CN 2836-32-0
PRO CO 73832-89-0

RX(44) OF 91 ...BX ==> CP



BX

(44) →



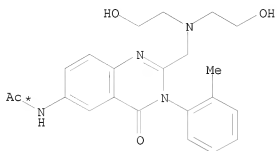
CP

RX(44) RCT BX 73832-71-0
RGT F 7647-01-0 HCl
PRO CP 73832-37-8

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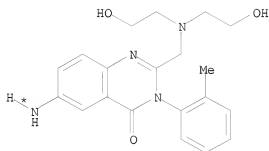
SOL 67-56-1 MeOH

RX(45) OF 91 ...CQ ==> CR



CQ

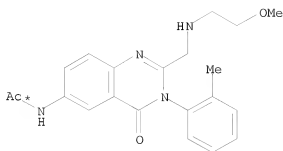
(45)
→



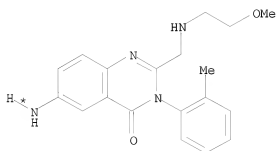
CR

RX(45) RCT CQ 73832-83-4
 RGT F 7647-01-0 HCl
 PRO CR 73832-41-4
 SOL 67-56-1 MeOH

RX(46) OF 91 ...CD ==> CS

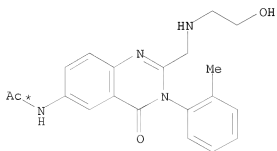


CD

(46) \longrightarrow 

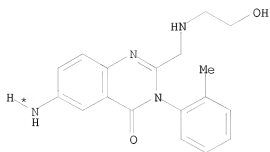
CS

RX (46)	RCT	CD 73832-84-5
	RGT	F 7647-01-0 HCl
	PRO	CS 73832-42-5
	SOL	67-56-1 MeOH

RX (47) OF 91 ...CF \implies CT

CF

(47) \longrightarrow

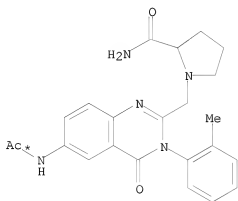


● 2 HCl

CT

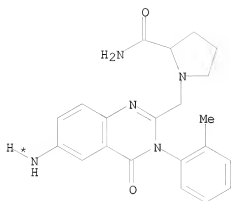
RX(47) RCT CF 73832-85-6
 RGT F 7647-01-0 HCl
 PRO CT 73832-43-6
 SOL 67-56-1 MeOH

RX(48) OF 91 ...CH ==> CU



CH

(48) $\xrightarrow{\hspace{1cm}}$

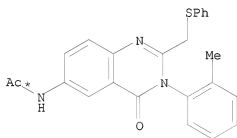


● 2 HCl

CU

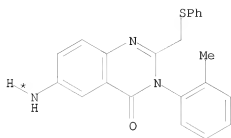
RX(48)	RCT	CH	73832-87-8
	RGT	F	7647-01-0 HCl
	PRO	CU	73832-45-8
	SOL	67-56-1	MeOH

RX(49) OF 91 ...CJ ==> CV



CJ

(49)
→

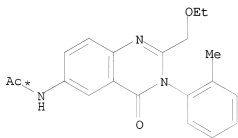


● HCl

CV

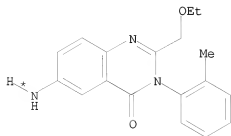
RX(49) RCT CJ 73832-73-2
 RGT F 7647-01-0 HCl
 PRO CV 73832-46-9
 SOL 67-56-1 MeOH

RX(50) OF 91 ...CW ==> CX



CW

(50) \Rightarrow

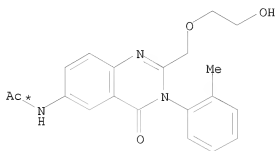


CX

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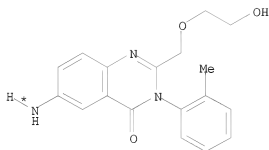
RX(50) RCT CW 73832-72-1
 RGT F 7647-01-0 HCl
 PRO CX 73832-48-1
 SOL 67-56-1 MeOH

RX(51) OF 91 ...CO ==> CY



CO

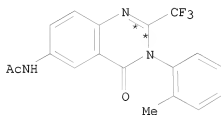
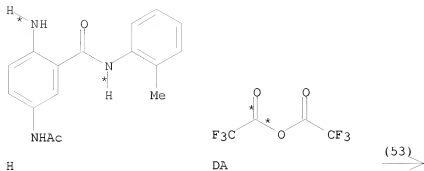
(51) \longrightarrow



CY

RX(51) RCT CO 73832-89-0
 RGT F 7647-01-0 HCl
 PRO CY 73832-90-3
 SOL 67-56-1 MeOH

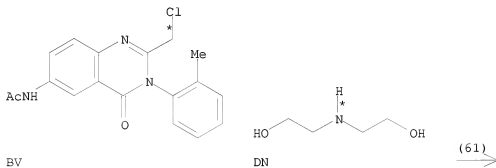
RX(53) OF 91 H + DA ==> D...



D

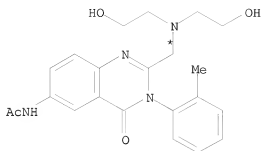
RX(53) RCT H 64102-81-4, DA 407-25-0
 RGT K 7637-07-2 BF₃
 PRO D 73832-50-5
 SOL 407-25-0 (CF₃CO)₂O, 60-29-7 Et₂O

RX(61) OF 91 BV + DN ==> CQ...



BV

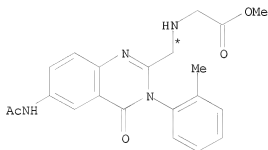
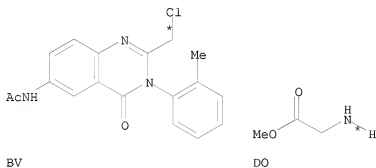
10/ 562,112



CQ

RX(61) RCT BV 61899-78-3, DN 111-42-2
 PRO CQ 73832-83-4
 SOL 109-99-9 THF

RX(62) OF 91 BV + DO ==> DP...

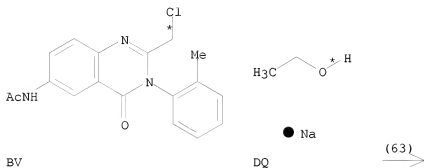


DP

RX(62) RCT BV 61899-78-3, DO 616-34-2
 PRO DP 73832-86-7
 SOL 109-99-9 THF

10/ 562,112

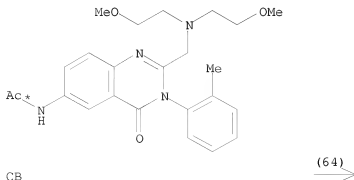
RX(63) OF 91 BV + DQ ==> CW...

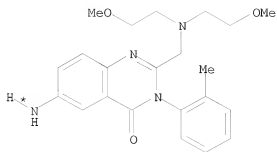


CW

RX(63) RCT BV 61899-78-3, DQ 141-52-6
 PRO CW 73832-72-1
 SOL 64-17-5 EtOH

RX(64) OF 91 ...CB ==> DS



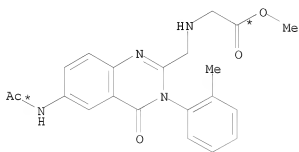


● 2 HCl

DS

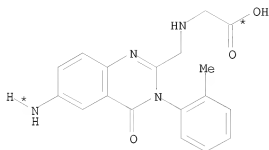
RX(64) RCT CB 73832-82-3
 RGT F 7647-01-0 HCl
 PRO DS 73832-40-3
 SOL 67-56-1 MeOH

RX(65) OF 91 ...DP ==> DT



DP

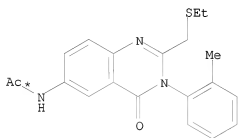
(65)
 →



DT

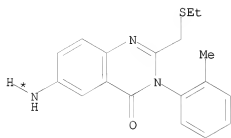
RX(65) RCT DP 73832-86-7
 RGT F 7647-01-0 HCl
 PRO DT 73832-44-7
 SOL 67-56-1 MeOH

RX(66) OF 91 ...CM ==> DU



CM

(66) →



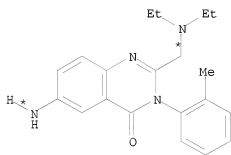
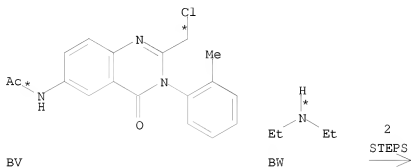
● HCl

DU

10/ 562,112

RX(66) RCT CM 73832-88-9
RGT F 7647-01-0 HCl
PRO DU 73832-47-0
SOL 67-56-1 MeOH

RX(77) OF 91 COMPOSED OF RX(35), RX(44)
RX(77) BV + BW ==> CP



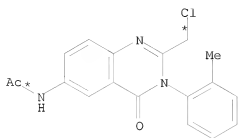
CP

RX(35) RCT BV 61899-78-3, BW 109-89-7
PRO BX 73832-71-0
SOL 109-99-9 THF

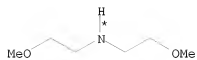
RX(44) RCT BX 73832-71-0
RGT F 7647-01-0 HCl
PRO CP 73832-37-8
SOL 67-56-1 MeOH

RX(78) OF 91 COMPOSED OF RX(37), RX(64)
RX(78) BV + CA ==> DS

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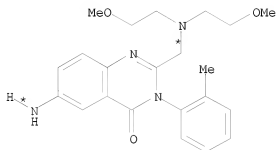


BV



CA

2
STEPS
→



● 2 HCl

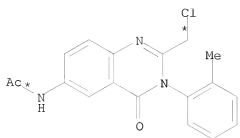
DS

RX(37) RCT BV 61899-78-3, CA 111-95-5
PRO CB 73832-82-3
SOL 109-99-9 THF

RX(64) RCT CB 73832-82-3
RGT F 7647-01-0 HCl
PRO DS 73832-40-3
SOL 67-56-1 MeOH

RX(79) OF 91 COMPOSED OF RX(38), RX(46)
RX(79) BV + CC ==> CS

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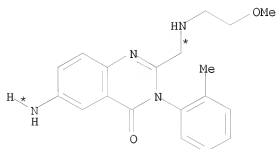


BV



CC

2
STEPS
→

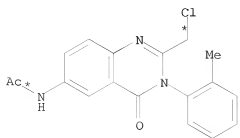


CS

RX(38) RCT BV 61899-78-3, CC 109-85-3
PRO CD 73832-84-5
SOL 109-99-9 THF

RX(46) RCT CD 73832-84-5
RGT F 7647-01-0 HCl
PRO CS 73832-42-5
SOL 67-56-1 MeOH

RX(80) OF 91 COMPOSED OF RX(39), RX(47)
RX(80) BV + CE ==> CT

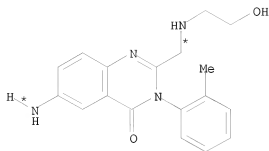


BV



CE

2
STEPS
→



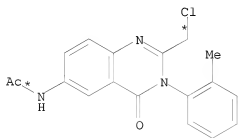
● 2 HCl

CT

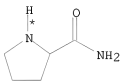
RX(39) RCT BV 61899-78-3, CE 141-43-5
 PRO CF 73832-85-6
 SOL 109-99-9 THF

RX(47) RCT CF 73832-85-6
 RGT F 7647-01-0 HCl
 PRO CT 73832-43-6
 SOL 67-56-1 MeOH

RX(81) OF 91 COMPOSED OF RX(40), RX(48)
 RX(81) BV + CG ==> CU

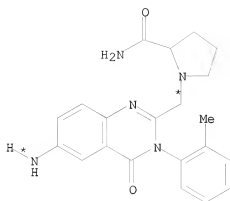


BV



CG

2
 STEPS
 →



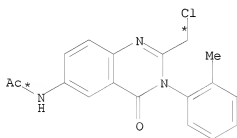
● 2 HCl

CU

RX(40) RCT BV 61899-78-3, CG 2812-47-7
 PRO CH 73832-87-8
 SOL 109-99-9 THF

RX(48) RCT CH 73832-87-8
 RGT F 7647-01-0 HCl
 PRO CU 73832-45-8
 SOL 67-56-1 MeOH

RX(82) OF 91 COMPOSED OF RX(41), RX(49)
 RX(82) BV + CI ==> CV

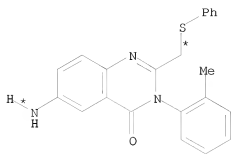


BV



CI

2
 STEPS
 >



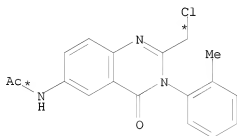
● HCl

CV

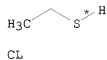
RX(41) RCT BV 61899-78-3, CI 108-98-5
 RGT CK 7646-69-7 NaH
 PRO CJ 73832-73-2
 SOL 109-99-9 THF

RX(49) RCT CJ 73832-73-2
 RGT F 7647-01-0 HCl
 PRO CV 73832-46-9
 SOL 67-56-1 MeOH

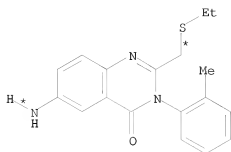
RX(83) OF 91 COMPOSED OF RX(42), RX(66)
 RX(83) BV + CL ==> DU



BV



2
 STEPS
 ➞



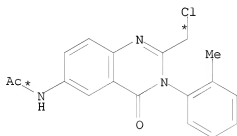
● HCl

DU

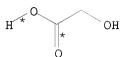
RX(42) RCT BV 61899-78-3, CL 75-08-1
 RGT CK 7646-69-7 NaH
 PRO CM 73832-88-9
 SOL 109-99-9 THF

RX(66) RCT CM 73832-88-9
 RGT F 7647-01-0 HCl
 PRO DU 73832-47-0
 SOL 67-56-1 MeOH

RX(84) OF 91 COMPOSED OF RX(43), RX(51)
 RX(84) BV + CN ==> CY



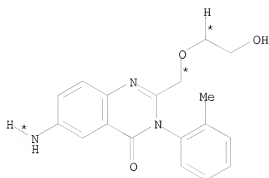
BV



● Na

CN

2
 STEPS
 ➞

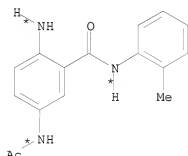


CY

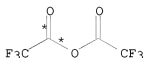
RX(43) RCT BV 61899-78-3, CN 2836-32-0
 PRO CO 73832-89-0

RX(51) RCT CO 73832-89-0
 RGT F 7647-01-0 HCl
 PRO CY 73832-90-3
 SOL 67-56-1 MeOH

RX(85) OF 91 COMPOSED OF RX(53), RX(2)
 RX(85) H + DA ==> E

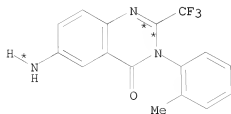


H



DA

2
 STEPS
 >



E

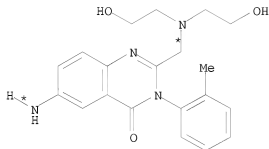
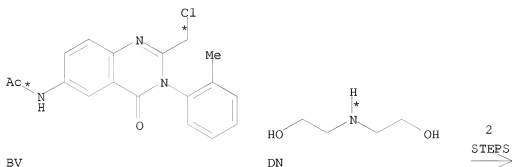
10/ 562,112

RX(53) RCT H 64102-81-4, DA 407-25-0
RGT K 7637-07-2 BF3
PRO D 73832-50-5
SOL 407-25-0 (CF3CO)2O, 60-29-7 Et2O

RX(2) RCT D 73832-50-5
RGT F 7647-01-0 HCl
PRO E 73832-08-3
SOL 67-56-1 MeOH

RX(88) OF 91 COMPOSED OF RX(61), RX(45)

RX(88) BV + DN ==> CR

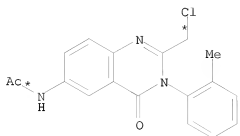


RX(61) RCT BV 61899-78-3, DN 111-42-2
PRO CQ 73832-83-4
SOL 109-99-9 THF

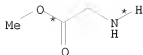
RX(45) RCT CQ 73832-83-4
RGT F 7647-01-0 HCl
PRO CR 73832-41-4
SOL 67-56-1 MeOH

RX(89) OF 91 COMPOSED OF RX(62), RX(65)

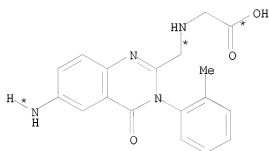
RX(89) BV + DO ==> DT



BV



DO

2
STEPS

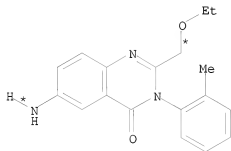
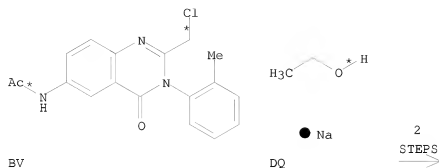
DT

RX(62) RCT BV 61899-78-3, DO 616-34-2
 PRO DP 73832-86-7
 SOL 109-99-9 THF

RX(65) RCT DP 73832-86-7
 RGT F 7647-01-0 HCl
 PRO DT 73832-44-7
 SOL 67-56-1 MeOH

RX(90) OF 91 COMPOSED OF RX(63), RX(50)

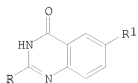
RX(90) BV + DQ ==> CX



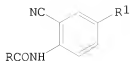
RX(63) RCT BV 61899-78-3, DQ 141-52-6
 PRO CW 73832-72-1
 SOL 64-17-5 EtOH

RX(50) RCT CW 73832-72-1
 RGT F 7647-01-0 HCl
 PRO CX 73832-48-1
 SOL 67-56-1 MeOH

L3 ANSWER 231 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 93:8126 CASREACT
 TITLE: A facile synthesis of
 2-substituted-4(3H)-quinazolinones
 AUTHOR(S): Showell, Graham A.
 CORPORATE SOURCE: Med. Res. Cent., Beecham Pharm., Harlow/Essex, CM19
 5AD, UK
 SOURCE: Synthetic Communications (1980), 10(3), 241-3
 CODEN: SYNCAV; ISSN: 0039-7911
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



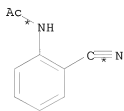
I



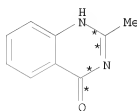
II

AB Quinazolones I (R = Me, R1 = H, NO₂, NH₂; R = Ph, R1 = H) were obtained in 85-97% yield by treating acylaminobenzonitriles II with 5N HCl at room temperature II (R = CF₃, R1 = H) did not cyclize under these conditions.

RX(2) OF 4 D ==> E

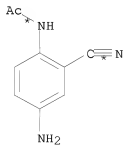


D

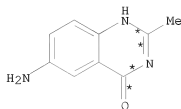
E
YIELD 91%

RX(2) RCT D 25116-00-1
RGT C 7647-01-0 HCl
PRO E 1769-24-0

RX(3) OF 4 F ==> G

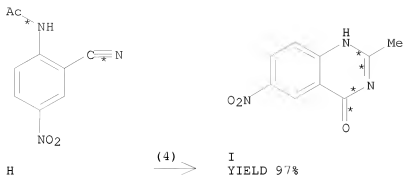


F

G
YIELD 85%

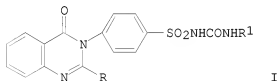
RX(3) RCT F 73894-39-0
RGT C 7647-01-0 HCl
PRO G 17329-24-7

RX(4) OF 4 H ==> I



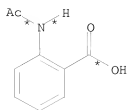
RX(4) RCT H 73894-38-9
 RGT C 7647-01-0 HCl
 PRO I 24688-36-6

L3 ANSWER 232 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 92:76439 CASREACT
 TITLE: Synthesis of substituted 4(3H)-quinazolinone
 sulfonylurea derivatives with possible antimicrobial
 or hypoglycemic effect
 AUTHOR(S): Soliman, Raafat
 CORPORATE SOURCE: Fac. Pharm., Univ. Alexandria, Alexandria, Egypt
 SOURCE: Pharmazie (1979), 34(7), 441-2
 CODEN: PHARAT; ISSN: 0031-7144
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

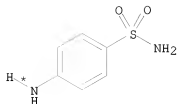


AB Sulfonylureas I (R = Me, Et; R1 = Et, Pr, Bu, cyclohexyl, CH2Ph, guanidino) were prepared by condensing 2-HO2CC6H4NHCOR with 4-H2NC6H4SO2NH2 and treating the resulting quinazolyphenylsulfonamides with R1NCO.

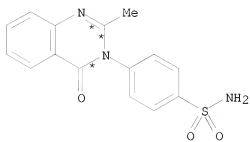
RX(1) OF 26 A + B ==> C...



A



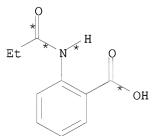
B

(1) \longrightarrow 

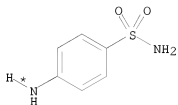
C

YIELD 80%

RX(1) RCT A 89-52-1, B 63-74-1
 PRO C 1232-38-8

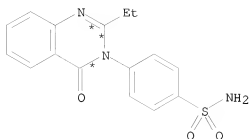
RX(2) OF 26 D + B \implies E...

D



B

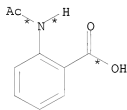
(2) \longrightarrow



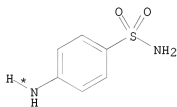
E
YIELD 85%

RX(2) RCT D 19165-26-5, B 63-74-1
PRO E 72723-65-0

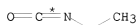
RX(14) OF 26 COMPOSED OF RX(1), RX(3)
RX(14) A + B + F ==> G



A

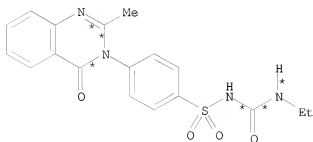


B



F

2
STEPS
→



G

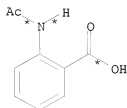
RX(1) RCT A 89-52-1, B 63-74-1

10/ 562,112

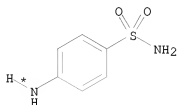
PRO C 1232-38-8

RX(3) RCT C 1232-38-8, F 109-90-0
PRO G 72723-66-1
CAT 584-08-7 K2CO3

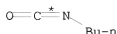
RX(15) OF 26 COMPOSED OF RX(1), RX(4)
RX(15) A + B + I ==> J



A

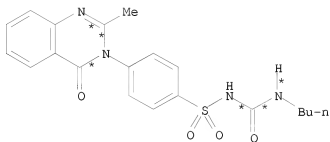


B



I

2
STEPS
=>



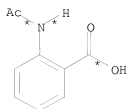
J

RX(1) RCT A 89-52-1, B 63-74-1
PRO C 1232-38-8

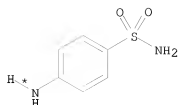
RX(4) RCT C 1232-38-8, I 111-36-4
PRO J 72723-68-3
CAT 584-08-7 K2CO3

RX(16) OF 26 COMPOSED OF RX(1), RX(5)
RX(16) A + B + K ==> L

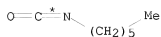
10/ 562,112



A

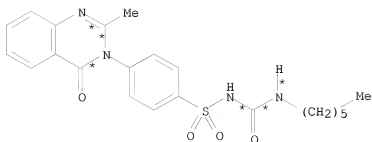


B



K

2
STEPS
→

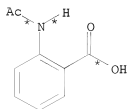


L

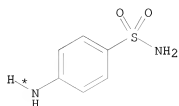
RX(1) RCT A 89-52-1, B 63-74-1
PRO C 1232-38-8

RX(5) RCT C 1232-38-8, K 2525-62-4
PRO L 343796-14-5
CAT 584-08-7 K2CO3

RX(17) OF 26 COMPOSED OF RX(1), RX(9)
RX(17) A + B + Q ==> R



A

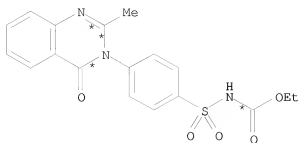


B



Q

2
STEPS
→

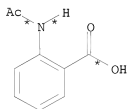


R

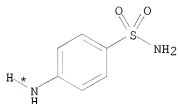
RX(1) RCT A 89-52-1, B 63-74-1
PRO C 1232-38-8

RX(9) RCT C 1232-38-8, Q 541-41-3
PRO R 72723-76-3
CAT 584-08-7 K2CO3

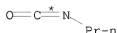
RX(18) OF 26 COMPOSED OF RX(1), RX(12)
RX(18) A + B + N ==> W



A

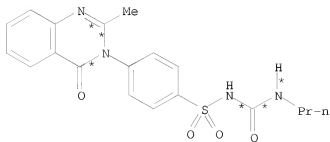


B



N

2
STEPS
→



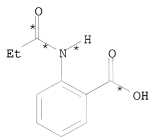
W

10/ 562,112

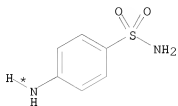
RX(1) RCT A 89-52-1, B 63-74-1
PRO C 1232-38-8

RX(12) RCT C 1232-38-8, N 110-78-1
PRO W 72723-67-2
CAT 584-08-7 K2CO3

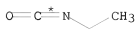
RX(19) OF 26 COMPOSED OF RX(2), RX(6)
RX(19) D + B + F ==> M



D

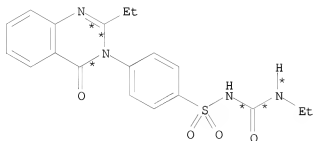


B



F

2
STEPS
=>

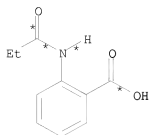


M

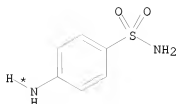
RX(2) RCT D 19165-26-5, B 63-74-1
PRO E 72723-65-0

RX(6) RCT E 72723-65-0, F 109-90-0
PRO M 72723-72-9
CAT 584-08-7 K2CO3

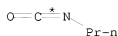
RX(20) OF 26 COMPOSED OF RX(2), RX(7)
RX(20) D + B + N ==> O



D

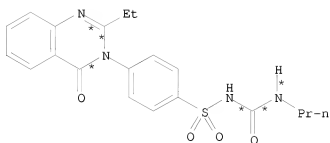


B



N

2
STEPS
→



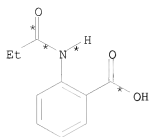
O

RX(2) RCT D 19165-26-5, B 63-74-1
PRO E 72723-65-0

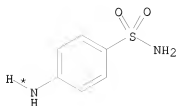
RX(7) RCT E 72723-65-0, N 110-78-1
PRO O 72723-73-0
CAT 584-08-7 K2C03

RX(21) OF 26 COMPOSED OF RX(2), RX(8)

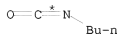
RX(21) D + B + I ==> P



D

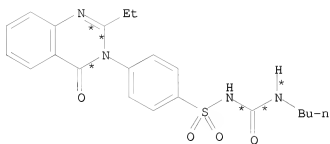


B



I

2
STEPS
→

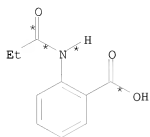


P

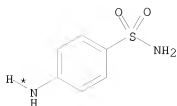
RX(2) RCT D 19165-26-5, B 63-74-1
PRO E 72723-65-0

RX(8) RCT E 72723-65-0, I 111-36-4
PRO P 72723-74-1
CAT 584-08-7 K2CO3

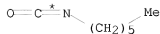
RX(22) OF 26 COMPOSED OF RX(2), RX(13)
RX(22) D + B + K ==> X



D

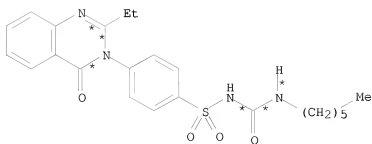


B



K

2
STEPS
→

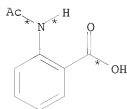


X

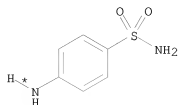
RX(2) RCT D 19165-26-5, B 63-74-1
PRO E 72723-65-0

RX(13) RCT E 72723-65-0, K 2525-62-4
PRO X 343796-84-9
CAT 584-08-7 K2CO3

RX(25) OF 26 COMPOSED OF RX(1), RX(9), RX(10)
RX(25) A + B + Q + S ==> T



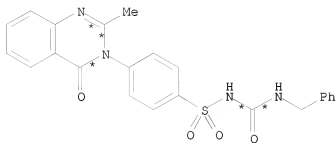
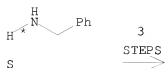
A



B



Q



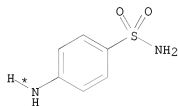
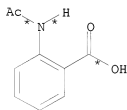
T
YIELD 72%

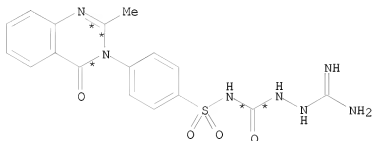
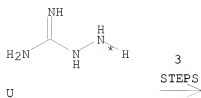
RX(1) RCT A 89-52-1, B 63-74-1
PRO C 1232-38-8

RX(9) RCT C 1232-38-8, Q 541-41-3
PRO R 72723-76-3
CAT 584-08-7 K2CO3

RX(10) RCT R 72723-76-3, S 100-46-9
PRO T 72723-70-7

RX(26) OF 26 COMPOSED OF RX(1), RX(9), RX(11)
RX(26) A + B + Q + U ==> V





V
YIELD 77%

RX(1) RCT A 89-52-1, B 63-74-1
PRO C 1232-38-8

RX(9) RCT C 1232-38-8, Q 541-41-3
PRO R 72723-76-3
CAT 584-08-7 K2CO3

RX(11) RCT R 72723-76-3, U 79-17-4
PRO V 72723-71-8

L3 ANSWER 233 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 92:58712 CASREACT

TITLE: Study in nitrogen mustards, Part III. Synthesis of some 2-alkyl-3-aryl-4 (3H)-quinazolinone derivatives with nitrogen mustard moiety as possible antitumor agents

AUTHOR(S): Singh, Pritpal; Gupta, I. S.

CORPORATE SOURCE: Dep. Chem. Eng. Technol., Panjab Univ., Chandigarh, 160 014, India

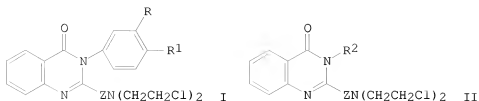
SOURCE: Journal of the Indian Chemical Society (1979), 56(1), 77-80

CODEN: JICSAH; ISSN: 0019-4522

DOCUMENT TYPE: Journal

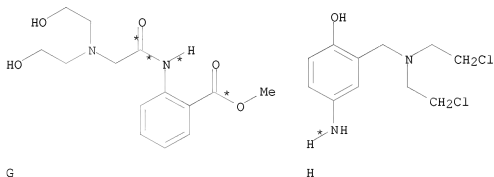
LANGUAGE: English

GI



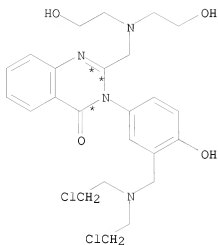
AB Title quinazolinones I [$Z = (CH_2)_n$ ($n = 0-2$), CHMe; $R =$ e.g. $CH_2N(CH_2CH_2OH)_2$, $CH_2NHCH_2CH_2Br$; $R_1 = OH, OMe, OEt$] (32 compds.) and II [$Z = (CH_2)_n$ ($n = 1, 2$), CHMe; $R_2 = CH_2CH_2N(CH_2CH_2X)_2$ ($X = Br, Cl, OH$), $SO_2C_6H_4N(CH_2CH_2Cl)_2$] (10 compds.) were prepared from N-acyl anthranilates by condensing with anilines or hydrazides, resp. I and II contain mono or bifunctional nitrogen mustard groups attached to the quinazoline through an enzymatically-hydrolyzable linkage; they showed relatively low toxicity.

RX(4) OF 12 ...G + H ==> I...



(4) →

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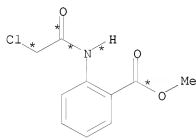
I

YIELD 60%

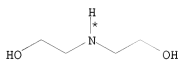
RX(4) RCT G 72544-39-9, H 56538-41-1
PRO I 72544-40-2

RX(8) OF 12 COMPOSED OF RX(3), RX(4)

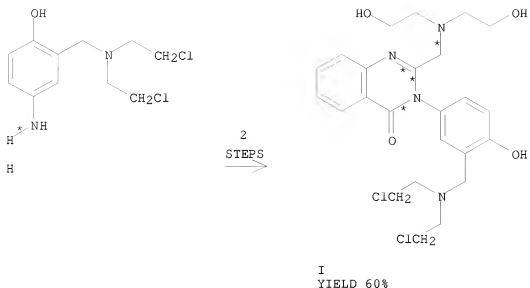
RX(8) E + F + H ==> I



E



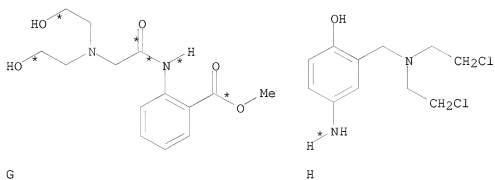
F



RX(3) RCT E 58915-18-7, F 111-42-2
PRO G 72544-39-9

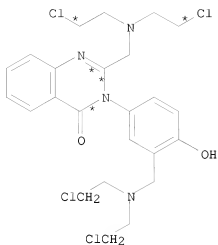
RX(4) RCT G 72544-39-9, H 56538-41-1
PRO I 72544-40-2

RX(9) OF 12 COMPOSED OF RX(4), RX(5)
RX(9) G + H ==> J



2
STEPS
→

10/ 562,112



J

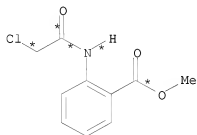
YIELD 57%

RX(4) RCT G 72544-39-9, H 56538-41-1
PRO I 72544-40-2

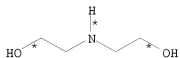
RX(5) RCT I 72544-40-2
RGT K 7719-09-7 SOC12
PRO J 72544-41-3

RX(11) OF 12 COMPOSED OF RX(3), RX(4), RX(5)

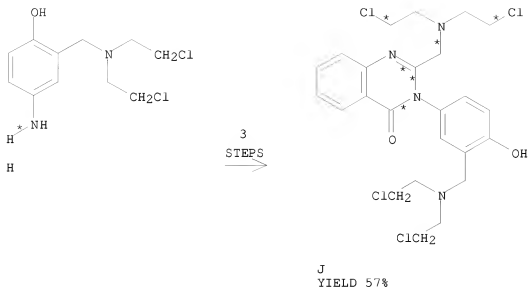
RX(11) E + F + H ==> J



E



F

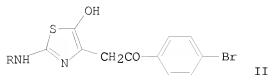


RX(3) RCT E 58915-18-7, F 111-42-2
PRO G 72544-39-9

RX(4) RCT G 72544-39-9, H 56538-41-1
PRO I 72544-40-2

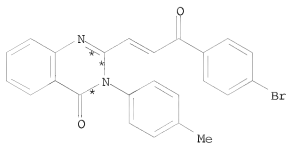
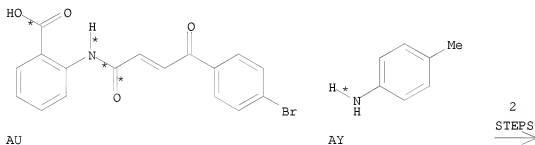
RX(5) RCT I 72544-40-2
RGT K 7719-09-7 SOCl₂
PRO J 72544-41-3

L3 ANSWER 234 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 92:41868 CASREACT
TITLE: Some reactions with β -(p-bromobenzoyl)acrylic acid
AUTHOR(S): Sammour, A.; Abdallah, M. M.; Essawy, A.; Elmobayed, M.
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
SOURCE: Egyptian Journal of Chemistry (1979), Volume Date 1976, 19(6), 911-26
CODEN: EGJCA3; ISSN: 0367-0422
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB 4-BrC6H4COCH:CHCO2H (I) reacted with piperidine to give α -(4-bromophenyl)-1-piperidineacetic acid; reaction of I with thioureas gave thiazoles II (R = H, CH2Ph, Ph), which were cyclized with N2H4 or NH2OH to give thiazolopyridazines and thiazolooxazines resp. Friedel-Crafts alkylation of R1Ph (R1 = H, Me, Et, CHMe2) with I gave 4-BrC6H4COCH2CH(CO2H)C6H4R-4 which, were cyclized to diarylfuranones with Ac2O or were condensed to pyridazinones with hydrazines or oxazinones with NH2OH. Michael reactions of I gave 4-BrC6H4COCH2CHR2CO2H [R2 = CH(CO2Et)2, CH(CO2Me)CH2CO2Me], which were hydrolyzed and decarboxylated to 4-BrC6H4COCH2CH(CO2H)CHR3CO2H (R3 = H, Me), which were cyclized to pyranones with Ac2O. 4-BrC6H4COCH:CHCOC1 (III) reacted with 2-H2NC6H4CO2H to give 2-HO2CC6H4NHCOC:CHCOC6H4Br-4, which was cyclized to the benzoxazinone with Ac2O. The benzoxazinone was cleaved by arylamines; III was also used to acylate sulfa drugs.

RX(55) OF 57 COMPOSED OF RX(29), RX(31)
 RX(55) AU + AY ==> AZ



AZ
 YIELD 85%

RX(29) RCT AU 71553-50-9

PRO AV 71553-51-0
CAT 108-24-7 Ac2O

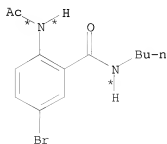
RX(31) RCT AV 71553-51-0, AY 106-49-0
PRO AZ 71553-53-2

L3 ANSWER 235 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 91:211360 CASREACT
TITLE: Some reactions with
6-bromo-2-methyl-4H-3,1-benzoxazin-4-one and
6-bromo-3-phenyl-2-methyl-4 (3H) -quinazolinone
AUTHOR(S): Sammour, A.; Rabie, A.; Elhashash, M.; Sayed, M.
CORPORATE SOURCE: Fac. Sci., Univ. Ain Shams, Cairo, Egypt
SOURCE: Egyptian Journal of Chemistry (1978), Volume Date
1976, 19(4), 571-88
CODEN: EGJCA3; ISSN: 0367-0422
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Aminolysis of I with RNH₂ (R = alkyl, aryl) gave the acetanilides II and quinazolinones III via cyclocondensation. Condensation of I with aromatic aldehydes, ketones, and anhydrides, or phthalimide gave 2-styrylbenzoxazinones (IV; R₁ = aryl), bisbromobenzoxazinones (V; R₂ = Me, Ph; R₃ = Me, Ph, PhCH₂), 1,3-diones (VI; R₄ = R₅ = H, R₄R₅ = benzo), and the benzopyrrolidone derivative VII, resp. Condensation of VI (R₄R₅ = benzo) with PhNH₂ and PhCH₂CO₂H gave VIII (Z = Z₁ = Z₂ = NPh and Z = Z₁ = O, Z₂ = CHPh, resp.). Condensation of I with hydrazines gave II (R = NH, arylamino), which was cyclized to III (R = NH₂, arylamino) by Ac₂O. Reaction of II (R = NH₂) with PhCHO gave III (R = PhCH:N) and with MeCOCO₂Et gave II (R = NHCCH₂COMe), which was cyclized to III (R = NHCCH₂COMe) by Ac₂O.

RX(6) OF 85 ...C + L ==> M



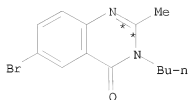
C



L



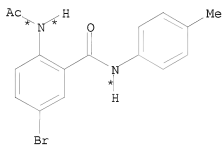
10/ 562,112



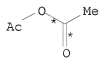
M
YIELD 78%

RX(6) RCT C 71822-55-4, L 108-24-7
PRO M 71822-61-2

RX(7) OF 85 ...E + L ==> N

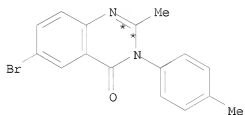


E



L

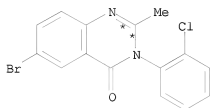
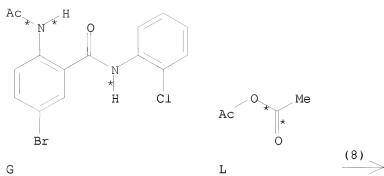
(7) ➞



N
YIELD 79%

RX(7) RCT E 71822-56-5, L 108-24-7
PRO N 71822-62-3

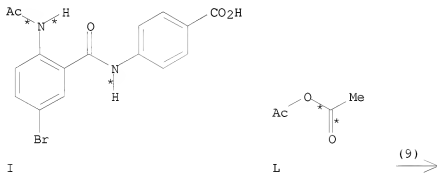
RX(8) OF 85 ...G + L ==> O



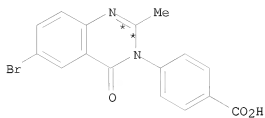
O
YIELD 77%

RX(8) RCT G 71822-57-6, L 108-24-7
PRO O 19868-06-5

RX(9) OF 85 ...I + L ==> P



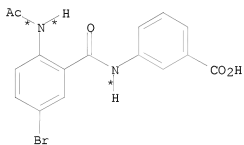
10/ 562,112



P
YIELD 81%

RX(9) RCT I 71822-58-7, L 108-24-7
PRO P 24295-50-9

RX(10) OF 85 ...K + L ==> Q

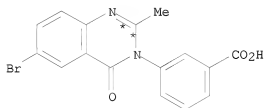


K



L

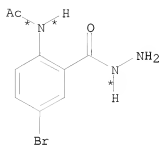
(10)
=>



Q
YIELD 79%

RX(10) RCT K 71822-59-8, L 108-24-7
PRO Q 72005-21-1

RX(33) OF 85 ...BG + L ==> BH...

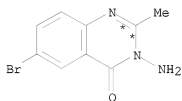


BG



L

(33)

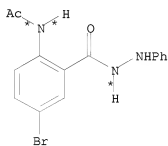


BH

YIELD 70%

RX(33) RCT BG 71822-95-2, L 108-24-7
PRO BH 71822-97-4

RX(34) OF 85 ...BD + L ==> BI



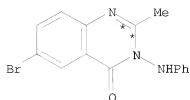
BD



L

(34)

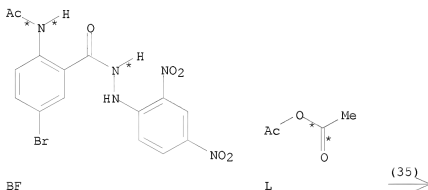
10/ 562,112



BI
YIELD 81%

RX(34) RCT BD 71822-96-3, L 108-24-7
PRO BI 71822-98-5

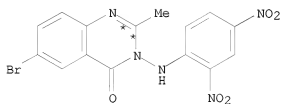
RX(35) OF 85 ...BF + L ==> BJ



BF

L

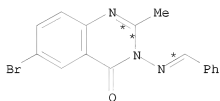
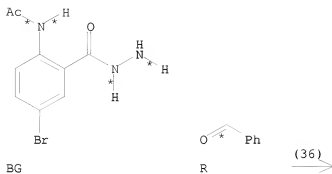
(35)



BJ
YIELD 79%

RX(35) RCT BF 71861-26-2, L 108-24-7
PRO BJ 71822-99-6

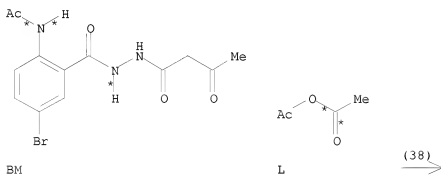
RX(36) OF 85 ...BG + R ==> BK



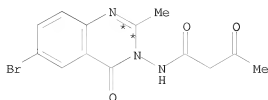
BK
YIELD 71%

RX(36) RCT BG 71822-95-2, R 100-52-7
PRO BK 71823-00-2

RX(38) OF 85 ...BM + L ==> BN



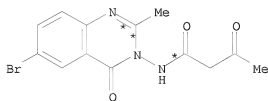
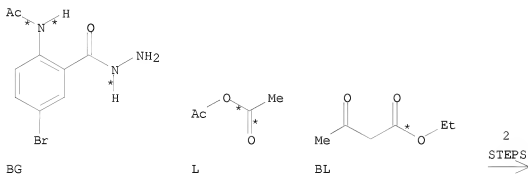
10/ 562,112



BN
YIELD 68%

RX(38) RCT BM 71823-01-3, L 108-24-7
PRO BN 71823-02-4

RX(57) OF 85 COMPOSED OF RX(33), RX(39)
RX(57) BG + L + BL ==> BN

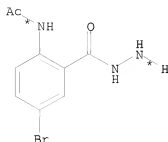


BN
YIELD 65%

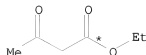
RX(33) RCT BG 71822-95-2, L 108-24-7
PRO BH 71822-97-4

RX(39) RCT BH 71822-97-4, BL 141-97-9
PRO BN 71823-02-4

RX(58) OF 85 COMPOSED OF RX(37), RX(38)
RX(58) BG + BL + L ==> BN



BG

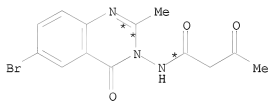


BL



L

2
STEPS
→

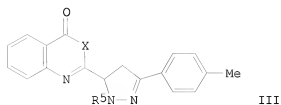
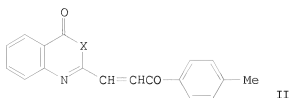


BN
YIELD 68%

RX(37) RCT BG 71822-95-2, BL 141-97-9
PRO BM 71823-01-3

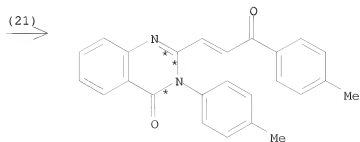
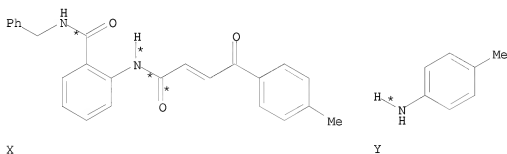
RX(38) RCT BM 71823-01-3, L 108-24-7
PRO BN 71823-02-4

L3 ANSWER 236 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 91:175295 CASREACT
 TITLE: Reactions with the amides and chlorides of some
 β-aroylacrylic acids
 AUTHOR(S): Sammour, A.; Afify, A. A.; Abdallah, M.; Soliman, E.
 A.
 CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt
 SOURCE: Egyptian Journal of Chemistry (1979), Volume Date
 1976, 19(6), 1109-16
 CODEN: EGJCA3; ISSN: 0367-0422
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB RCOCH:CHCONHCSNHR1 (R = 4-MeC6H4, 2-naphthyl; R1 = H, CH2Ph) were prepared by treating RCOCH:CHCONHC6H4R2-4 (R2 = H, Me, OMe) or 4-MeC6H4COCH:CHCOCl (I) with H2NCSNHR1. 4-MeC6H4COCH:CHCONHC6H4SO2NHR3-4 (R3 = H, C(:NH)NH2, 4-methyl-2-pyrimidinyl) were obtained from I and H2NC6H4SO2NHR3-4. I reacted with 2-H2NC6H4CO2H to give 2-HO2CC6H4NHCOCCH:CHCOC6H4Me-4, which cyclized to the benzoxazinone II (X = O). Reaction of II (X = O) with amines R4NH2 in EtOH gave 2-R4NHCOC6H4NHCOCCH:CHCOC6H4Me-4 (R4 = CH2Ph, 4-MeC6H4), but reaction with 4-MeC6H4NH2 at 170° gave II (X = NC6H4Me-4). Reaction of II (X = O) with N2H4 gave III (X = O, NNH2, R5 = H), whereas with PhNHNH2 only III (X = NNHPh, R5 = Ph) was obtained.

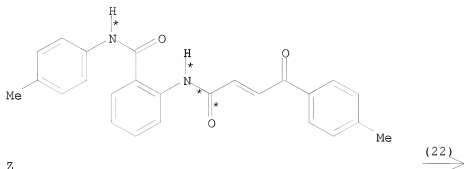
RX(21) OF 37 ...X + Y ==> AA



10/ 562,112

RX(21) RCT X 71703-79-2, Y 106-49-0
 PRO AA 71703-81-6

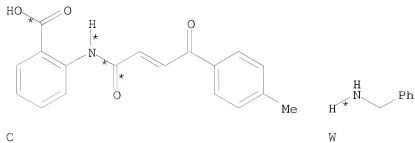
RX(22) OF 37 ...Z ==> AA

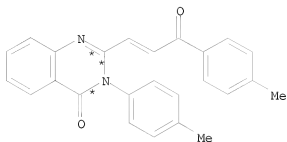
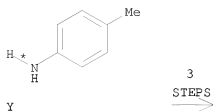


AA

RX(22) RCT Z 71703-80-5
 PRO AA 71703-81-6
 CAT 106-49-0 4-MeC₆H₄NH₂

RX(34) OF 37 COMPOSED OF RX(18), RX(19), RX(21)
 RX(34) C + W + Y ==> AA



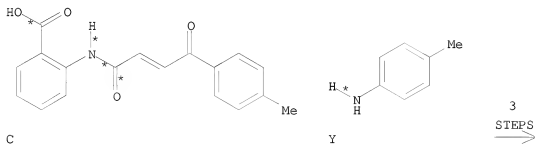


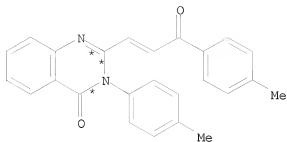
RX(18) RCT C 70596-64-4
 PRO U 71703-78-1
 CAT 108-24-7 Ac2O

RX(19) RCT U 71703-78-1, W 100-46-9
 PRO X 71703-79-2

RX(21) RCT X 71703-79-2, Y 106-49-0
 PRO AA 71703-81-6

RX(35) OF 37 COMPOSED OF RX(18), RX(20), RX(22)
 RX(35) C + Y ==> AA





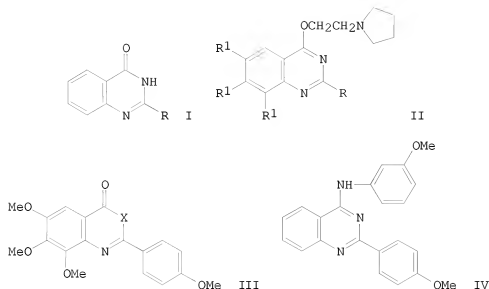
AA

RX(18) RCT C 70596-64-4
 PRO U 71703-78-1
 CAT 108-24-7 Ac2O

 RX(20) RCT U 71703-78-1, Y 106-49-0
 PRO Z 71703-80-5

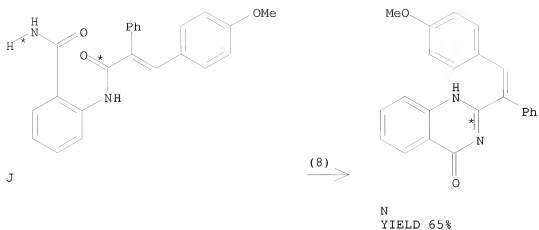
 RX(22) RCT Z 71703-80-5
 PRO AA 71703-81-6
 CAT 106-49-0 4-MeC6H4NH2

L3 ANSWER 237 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 91:157681 CASREACT
 TITLE: Heterocyclic compounds. XII. Quinazoline derivatives
 as potential antifertility agents
 AUTHOR(S): Manhas, M. S.; Hoffman, W. A., III; Bose, A. K.
 CORPORATE SOURCE: Dep. Chem. Chem. Eng., Stevens Inst. Technol.,
 Hoboken, NJ, 07030, USA
 SOURCE: Journal of Heterocyclic Chemistry (1979), 16(4),
 711-15
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



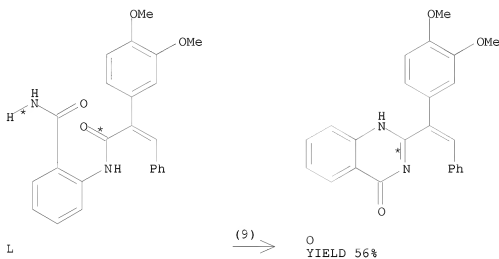
AB Acylation of 2-H₂NC₆H₄CONH₂ by RCOC₁ [R = 4-MeOC₆H₄, 4-MeOC₆H₄CH:CPh, α-benzylidene-3,4-dimethoxybenzyl, 3,4-methylenedioxyphenyl] gave 2-(RCONH)C₆H₄CONH₂, which cyclized in refluxing Ph₂O to give the corresponding quinazolinones I. Chlorination of I by POCl₃ followed by substitution reaction with 2-pyrrolidinoethanol Na salt gave ethoxyquinazolines II (R as defined above; R₁ = H). Hydrogenation of Me 3,4,5-trimethoxy-2-nitrobenzoate over Pt/C followed by acylation with 4-MeOC₆H₄COCl gave Me 2-(p-methoxybenzamido)-3,4,5-trimethoxybenzoate, which underwent cyclocondensation in refluxing C₆H₆ containing NaOMe to give the benzoxazinone III (X = O). Treatment of III (X = O) with NH₃ in MeOH under pressure gave III (X = NH), which underwent chlorination and substitution reaction with pyrrolidinoethanol Na salt to give II (R = 4-MeOC₆H₄; R₁ = MeO). Reaction of I (R = 4-MeOC₆H₄) with P₂S₅ gave the corresponding quinazolinethione, which underwent S-methylation with Me iodide and then substitution reaction with 3-MeOC₆H₄NH₂ to give the anilinoquinazoline IV. II (R = 4-MeOC₆H₄, α-benzylidene-3,4,5-trimethoxybenzyl, 3,4-methylenedioxyphenyl; R₁ = H) and IV possessed low level postcoital contraceptive activity in rats.

RX(8) OF 82 ...J ==> N...



RX(8) RCT J 71628-56-3
 PRO N 344878-36-0

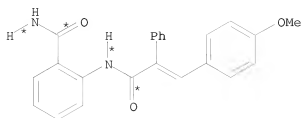
RX(9) OF 82 ...L ==> O...



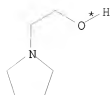
RX(9) RCT L 344878-90-6
 PRO O 344878-48-4

RX(66) OF 82 COMPOSED OF RX(8), RX(10), RX(14)
 RX(66) J + U ==> W

10/ 562,112



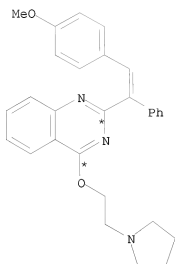
J



U

● Na

3
STEPS
→



W

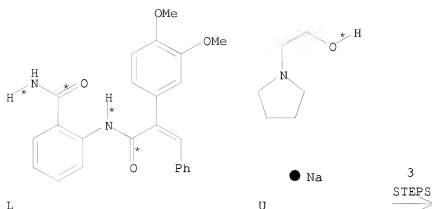
YIELD 37%

RX(8) RCT J 71628-56-3
PRO N 344878-36-0

RX(10) RCT N 344878-36-0
RGT Q 10025-87-3 POC13
PRO P 344878-35-9

RX(14) RCT P 344878-35-9, U 71628-68-7
PRO W 344909-05-3

RX(68) OF 82 COMPOSED OF RX(9), RX(11), RX(15)
RX(68) L + U ==> X



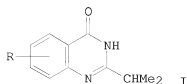
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(9) RCT L 344878-90-6
PRO O 344878-48-4

RX(11) RCT O 344878-48-4
RGT Q 10025-87-3 POC13
PRO R 344878-46-2

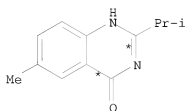
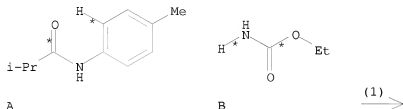
RX(15) RCT R 344878-46-2, U 71628-68-7
PRO X 344909-41-7

L3 ANSWER 238 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 91:123700 CASREACT
 TITLE: Studies in quinazolones: Part I. Synthesis and
 spectral characteristics of substituted
 2-isopropyl-4(3H)-quinazolones
 AUTHOR(S): Joshi, B. P.; Hosangadi, B. D.
 CORPORATE SOURCE: Dep. Chem., Univ. Bombay, Bombay, 400098, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic
 Chemistry Including Medicinal Chemistry (1978),
 16B(12), 1067-72
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Approx. 10 2-isopropyl-4(3H)-quinazolones (I, R = Me, OMe, OEt, benzo) and their corresponding N-Me derivs. were synthesized by cyclization of EtO₂CNH₂ with isobutyranilides, and their UV, IR and PMR spectral data discussed. Direct oxidation of 2-isopropyl-6-methyl-4(3H)-quinazolone with H₂O₂-AcOH gave 2-acetoxyisopropyl-6-methyl-4(3H)-quinazolone. This was the first acetoxylation of heterocyclic N-oxides in aqueous medium.

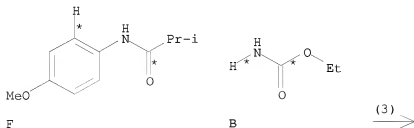
RX(1) OF 33 A + B ==> C...



C

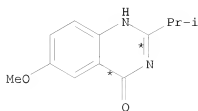
RX(1) RCT A 6876-49-9, B 51-79-6
PRO C 71182-14-4

RX(3) OF 33 F + B ==> G...



F

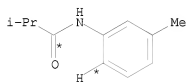
B



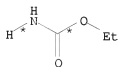
G

RX(3) RCT F 6642-37-1, B 51-79-6
PRO G 71182-16-6

RX(6) OF 33 K + B ==> L...

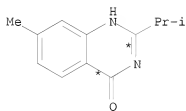


K



B

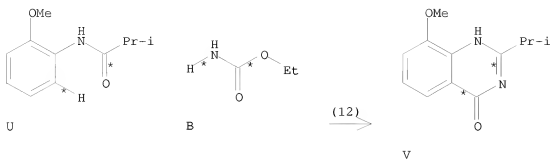
(6) ➞



L

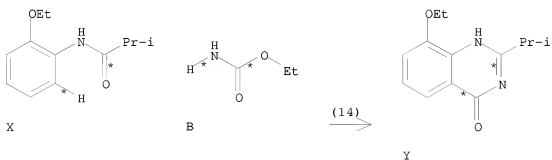
RX(6) RCT K 7146-00-1, B 51-79-6
PRO L 71182-20-2

RX(12) OF 33 U + B ==> V...



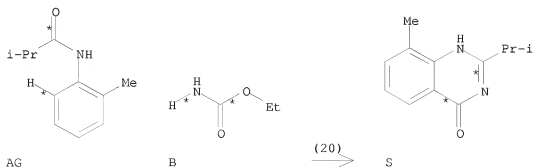
RX(12) RCT U 71182-38-2, B 51-79-6
PRO V 71182-27-9

RX(14) OF 33 X + B \implies Y...



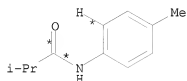
RX(14) RCT X 71182-39-3, B 51-79-6
PRO Y 71182-29-1

RX(20) OF 33 AG + B \implies S...

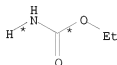


RX(20) RCT AG 55577-63-4, B 51-79-6
PRO S 71381-27-6

RX(23) OF 33 COMPOSED OF RX(1), RX(2)
 RX(23) A + B + D ==> E



A

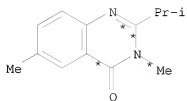


B



D

2
STEPS
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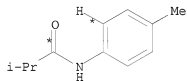


E

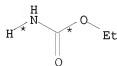
RX(1) RCT A 6876-49-9, B 51-79-6
 PRO C 71182-14-4

RX(2) RCT C 71182-14-4, D 74-88-4
 PRO E 71182-15-5

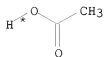
RX(24) OF 33 COMPOSED OF RX(1), RX(22)
 RX(24) A + B + AI ==> AJ



A

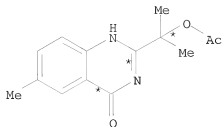


B



AI

2
STEPS
→

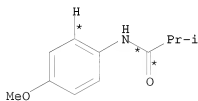


AJ

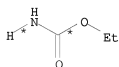
RX(1) RCT A 6876-49-9, B 51-79-6
PRO C 71182-14-4

RX(22) RCT C 71182-14-4, AI 64-19-7
RGT AK 7722-84-1 H202
PRO AJ 71182-35-9

RX(25) OF 33 COMPOSED OF RX(3), RX(4)
RX(25) F + B + D ==> H



F

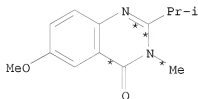


B



D

2
STEPS
→

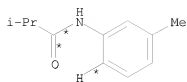


H

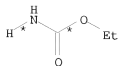
RX(3) RCT F 6642-37-1, B 51-79-6
PRO G 71182-16-6

RX(4) RCT G 71182-16-6, D 74-88-4
PRO H 71182-17-7

RX(26) OF 33 COMPOSED OF RX(6), RX(19)
RX(26) K + B + D ==> AF



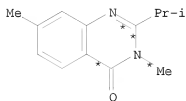
K



B



D

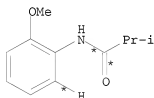


AF

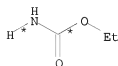
RX(6) RCT K 7146-00-1, B 51-79-6
PRO L 71182-20-2

RX(19) RCT L 71182-20-2, D 74-88-4
PRO AF 71182-21-3

RX(29) OF 33 COMPOSED OF RX(12), RX(13)
RX(29) U + B + D ==> W



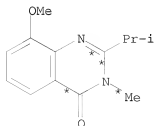
U



B



D



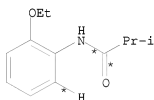
W

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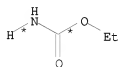
RX(12) RCT U 71182-38-2, B 51-79-6
PRO V 71182-27-9

RX(13) RCT V 71182-27-9, D 74-88-4
PRO W 71182-28-0

RX(30) OF 33 COMPOSED OF RX(14), RX(15)
RX(30) X + B + D ==> Z



X

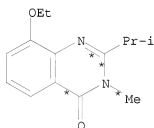


B



D

2
STEPS
→

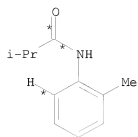


Z

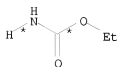
RX(14) RCT X 71182-39-3, B 51-79-6
PRO Y 71182-29-1

RX(15) RCT Y 71182-29-1, D 74-88-4
PRO Z 71182-30-4

RX(32) OF 33 COMPOSED OF RX(20), RX(11)
RX(32) AG + B + D ==> T



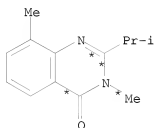
AG



B



D



T

RX(20) RCT AG 55577-63-4, B 51-79-6
PRO S 71381-27-6

RX(11) RCT S 71381-27-6, D 74-88-4
PRO T 71182-26-8

L3 ANSWER 239 OF 258 CASREACT COPYRIGHT 2009 ACS on SIN

ACCESSION NUMBER: 90:152149 CASREACT

TITLE: Studies on the synthesis of heterocyclic compounds.
Part II. Action of phosphorus oxychloride on
N-methyl-N-(1-phenyl-3-methylpyrazol-5-yl)-2-
acetamidobenzamide

AUTHOR(S): Plescia, S.; Daidone, G.; Sprio, V.; Aiello, E.;
Dattolo, G.; Cirrincione, G.

CORPORATE SOURCE: Ist. Chim. Farm., Univ. Studi Palermo, Palermo, Italy
SOURCE: Journal of Heterocyclic Chemistry (1978), 15(8),
1339-42

CODEN: JHTCAD; ISSN: 0022-152X

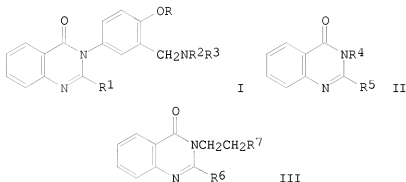
DOCUMENT TYPE: Journal

LANGUAGE: English

GI

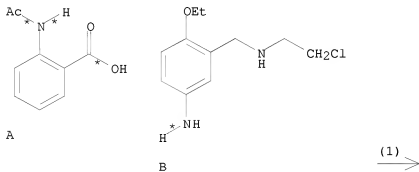
DOCUMENT TYPE:
LANGUAGE:
GI

Journal
English

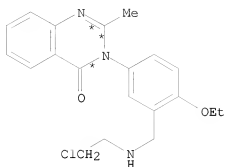


AB Quinazolinone mustards I (R = H, Me, Et; R1 = H, Me; R2, R3 = H, CH2CH2Cl, CH2CH2Br) (25 compds.), II [R4 = (ClCH2CH2)2NC6H4SO2, (HOCH2CH2)2N, (ClCH2CH2)2N, (BrCH2CH2)2N, (ClCH2CH2)2NC6H4; R5 = H, Me] (9 compds.), and III [R6 = H, Me; R7 = (HOCH2CH2)2N, (ClCH2CH2)2N, (BrCH2CH2)2N, [(ClCH2CH2)2NCH2](R8O)C6H3NH (R8 = H, Me, Et)] (13 compds.) were prepared and possess activity against lymphoid leukemia L1210 in preliminary screening. Thus, cyclocondensation of 2-(AcNH)C6H4CO2Me with 2,5-(EtO)(H2N)C6H3CH2N(CH2CH2Cl)2 gave 75% I (R = Et, R1 = Me, R2 = R3 = ClCH2CH2). Amination of III (R6 = Me, R7 = Cl) with (BrCH2CH2)2NH gave 80% III (R6 = Me, R7 = (BrCH2CH2)2N).

RX(1) OF 23 A + B ==> C



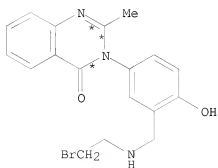
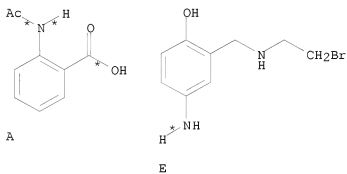
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C
YIELD 57%

RX(1) RCT A 89-52-1, B 56538-52-4
 RGT D 7789-60-8 PBr3
 PRO C 69561-23-5

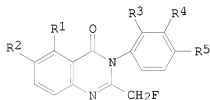
RX(2) OF 23 A + E ==> F



F
YIELD 62%

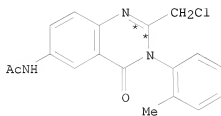
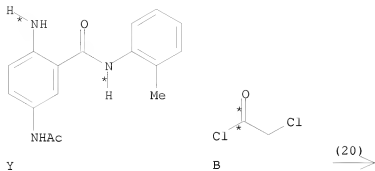
RX(2) RCT A 89-52-1, E 69561-59-7
 RGT D 7789-60-8 PBr3
 PRO F 69561-24-6

L3 ANSWER 241 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 90:80710 CASREACT
 TITLE: Studies on biologically active halogenated compounds.
 1. Synthesis and central nervous system depressant
 activity of 2-(fluoromethyl)-3-aryl-4(3H)-
 quinazolinone derivatives
 AUTHOR(S): Tani, Junichi; Yamada, Yoshihisa; Oine, Toyonari;
 Ochiai, Takashi; Ishida, Ryuichi; Inoue, Ichizo
 CORPORATE SOURCE: Res. Lab., Tanabe Seiyaku Co., Ltd., Osaka, Japan
 SOURCE: Journal of Medicinal Chemistry (1979), 22(1), 95-9
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The title compds. I (R1 = H or Cl; R2 = H, Cl, NH2, NO2 or NHAc; R3 = H, Cl, or Me; R4 and R5 = H or Cl) were prepared by the reaction of the appropriate anthranilic acid derivative with SOCl2 followed by treatment with anilines, chloroacetylation of the formed anthranilanilides and their cyclization followed by displacement of Cl by F. CNS activities of I were compared to methaqualone and 6-aminomethaqualone.
 3-(3-Chloro-o-tolyl)-2-(fluoromethyl)-4-(3H)-quinazolinone [49700-31-4] was more potent in CNS depressant activity and less toxic than methaqualone. Structure-activity relations are discussed.

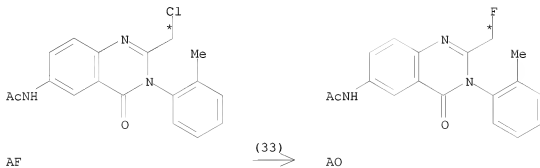
RX(20) OF 78 ...Y + B ==> AF...



AF
YIELD 81%

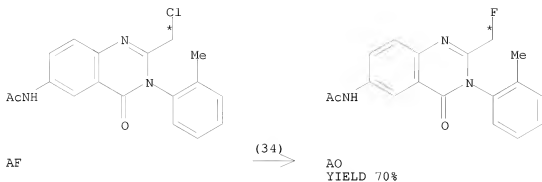
RX(20) RCT Y 64102-81-4, B 79-04-9
PRO AF 61899-78-3

RX(33) OF 78 ...AF ==> AO...



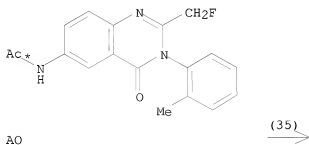
RX(33) RCT AF 61899-78-3
RGT I 7789-23-3 KF
PRO AO 61899-79-4

RX(34) OF 78 AF ==> AO



RX(34) RCT AF 61899-78-3
PRO AO 61899-79-4

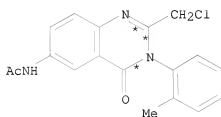
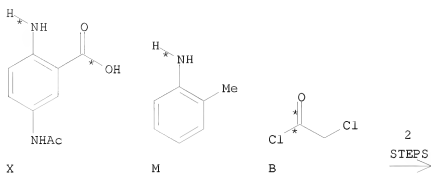
RX(35) OF 78 ...AO ==> AP



AP
YIELD 61%

RX(35) RCT AO 61899-79-4
PRO AP 56287-74-2

RX(51) OF 78 COMPOSED OF RX(13), RX(20)
RX(51) X + M + B ==> AF

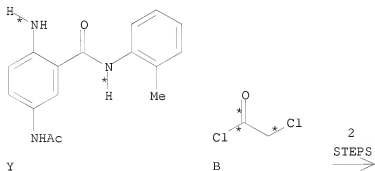


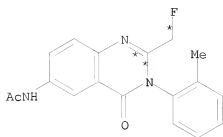
AF
YIELD 81%

RX(13) RCT X 50670-83-2, M 95-53-4
PRO Y 64102-81-4

RX(20) RCT Y 64102-81-4, B 79-04-9
PRO AF 61899-78-3

RX(58) OF 78 COMPOSED OF RX(20), RX(33)
RX(58) Y + B \implies AO



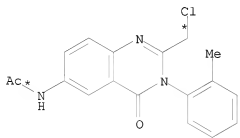


AO

RX(20) RCT Y 64102-81-4, B 79-04-9
PRO AF 61899-78-3

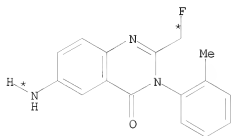
RX(33) RCT AF 61899-78-3
RGT I 7789-23-3 KF
PRO AO 61899-79-4

RX(60) OF 78 COMPOSED OF RX(33), RX(35)
RX(60) AF ==> AP



AF

2
STEPS
→



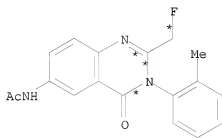
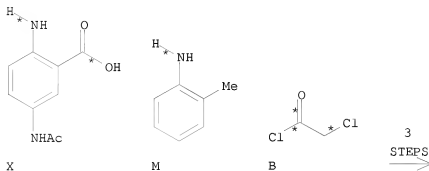
AP
YIELD 61%

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RX(33) RCT AF 61899-78-3
 RGT I 7789-23-3 KF
 PRO AO 61899-79-4

RX(35) RCT AO 61899-79-4
 PRO AP 56287-74-2

RX(72) OF 78 COMPOSED OF RX(13), RX(20), RX(33)
 RX(72) X + M + B ==> AO



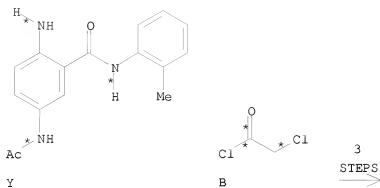
AO

RX(13) RCT X 50670-83-2, M 95-53-4
 PRO Y 64102-81-4

RX(20) RCT Y 64102-81-4, B 79-04-9
 PRO AF 61899-78-3

RX(33) RCT AF 61899-78-3
 RGT I 7789-23-3 KF
 PRO AO 61899-79-4

RX(75) OF 78 COMPOSED OF RX(20), RX(33), RX(35)
 RX(75) Y + B ==> AP



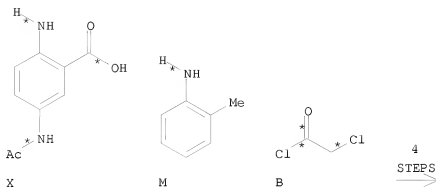
AP
YIELD 61%

RX(20) RCT Y 64102-81-4, B 79-04-9
PRO AF 61899-78-3

RX(33) RCT AF 61899-78-3
RGT I 7789-23-3 KF
PRO AO 61899-79-4

RX(35) RCT AO 61899-79-4
PRO AP 56287-74-2

RX(76) OF 78 COMPOSED OF RX(13), RX(20), RX(33), RX(35)
RX(76) X + M + B ==> AP



AP
YIELD 61%

RX(13) RCT X 50670-83-2, M 95-53-4
PRO Y 64102-81-4

RX(20) RCT Y 64102-81-4, B 79-04-9
PRO AF 61899-78-3

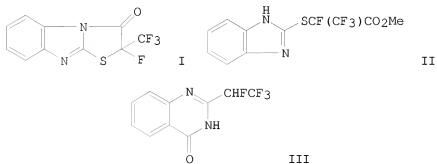
RX(33) RCT AF 61899-78-3
RGT I 7789-23-3 KF
PRO AO 61899-79-4

RX(35) RCT AO 61899-79-4
PRO AP 56287-74-2

L3 ANSWER 242 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 90:38837 CASREACT
TITLE: Preparation of fluorinated imidazole derivatives using
hexafluoro-1,2-epoxypropane
AUTHOR(S): Hammouda, Hamdy A.; Ishikawa, Nobuo
CORPORATE SOURCE: Dep. Chem. Technol., Tokyo Inst. Technol., Tokyo,
Japan
SOURCE: Bulletin of the Chemical Society of Japan (1978),
51(10), 3091-2

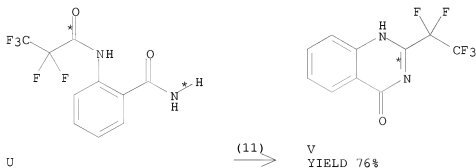
DOCUMENT TYPE:
LANGUAGE:
GI

CODEN: BCSJA8; ISSN: 0009-2673
Journal
English



AB Utilizing the reactivity of hexafluoro-1,2-epoxypropane, several new fluorine-containing imidazole derivs., e.g. I, II, and III, were prepared by reactions with 2-mercaptobenzimidazole, and o-H2NC6H4CONH2.

RX(11) OF 12 ...U ==> V

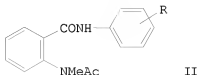
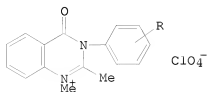


RX(11) RCT U 68790-62-5
PRO V 35982-15-1

L3 ANSWER 243 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 89:43305 CASREACT
TITLE: Study of 4(3H)-quinazolinones. IX. Synthesis and biological activity of 1,2-dimethyl-3-aryl-4(3H)-quinazolinonium perchlorates
AUTHOR(S): Zalesov, V. S.; Kozhevnikov, Yu. V.; Pilat, V. S.; Gradel, I. I.
CORPORATE SOURCE: Perm. Farm. Inst., Perm., USSR
SOURCE: Izuch. Biol. Deistviya Nov. Prod. Org. Sint. Prir. Soedin. (1977), 131-6. Editor(s): Pidemskii, E. L. Permsk. Gos. Univ. im. A. M. Gor'kogo: Perm, USSR.

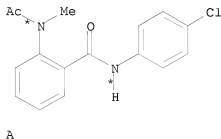
DOCUMENT TYPE:
LANGUAGE:
GI

CODEN: 37YKA4
Conference
Russian

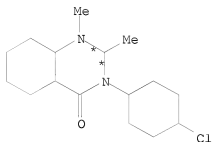


AB The title compds. I (R = H, 2-, 3-, 4-Me, 2-, 4-Cl, 2-, 3-, 4-Br, 4-MeO, 4-EtO), useful as antispasmodics, were prepared in 64-90% yields by cyclization of II, prepared in 48-80% yields by acetylation of the corresponding amine, with HClO₄.

RX(1) OF 11 A ==> B



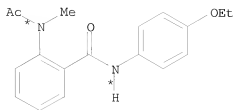
B: CM 1
YIELD 83%



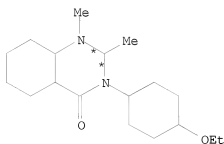
B: CM 2
YIELD 83%

RX(1) RCT A 66860-37-5
RGT C 7601-90-3 HClO₄
PRO B 66860-54-6

RX(2) OF 11 D ==> E

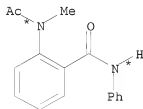


D

E: CM 1
YIELD 74%E: CM 2
YIELD 74%

RX(2) RCT D 66860-42-2
RGT C 7601-90-3 HClO4
PRO E 66860-63-7

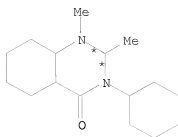
RX(3) OF 11 F ==> G



F

G: CM 1
YIELD 65%

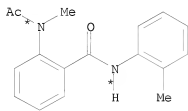
10/ 562,112



G: CM 2
YIELD 65%

RX(3) RCT F 66860-32-0
 RGT C 7601-90-3 HC104
 PRO G 66860-44-4

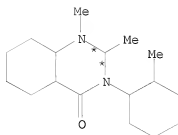
RX(4) OF 11 H ==> I



H



I: CM 1
YIELD 74%

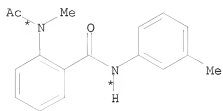


I: CM 2
YIELD 74%

RX(4) RCT H 66860-33-1
 RGT C 7601-90-3 HC104
 PRO I 66860-46-6

10/ 562,112

RX(5) OF 11 J ==> K

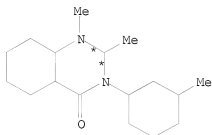


J

(5) →



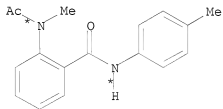
K: CM 1
YIELD 60%



K: CM 2
YIELD 60%

RX(5) RCT J 66860-34-2
RGT C 7601-90-3 HC104
PRO K 66860-48-8

RX(6) OF 11 L ==> M



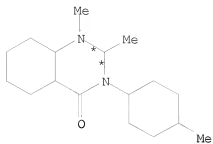
L

(6) →



M: CM 1
YIELD 80%

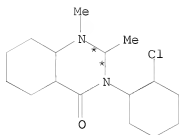
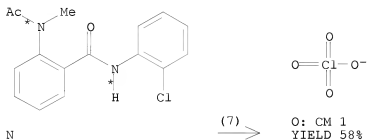
10/ 562,112



M: CM 2
YIELD 80%

RX(6) RCT L 66860-35-3
 RGT C 7601-90-3 HC104
 PRO M 66860-50-2

RX(7) OF 11 N ==> O

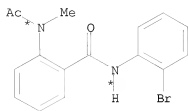


O: CM 2
YIELD 58%

RX(7) RCT N 66860-36-4
 RGT C 7601-90-3 HC104
 PRO O 66860-52-4

10/ 562,112

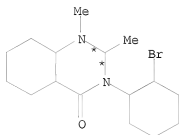
RX(8) OF 11 P ==> Q



P



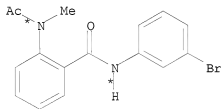
Q: CM 1
YIELD 64%



Q: CM 2
YIELD 64%

RX(8) RCT P 66860-38-6
RGT C 7601-90-3 HClO4
PRO Q 66860-55-7

RX(9) OF 11 R ==> S

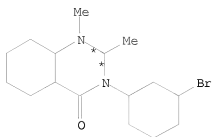


R



S: CM 1
YIELD 70%

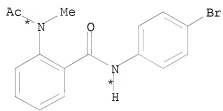
10/ 562,112



S: CM 2
YIELD 70%

RX(9) RCT R 66860-39-7
 RGT C 7601-90-3 HC104
 PRO S 66860-57-9

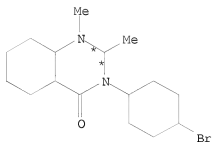
RX(10) OF 11 T ==> U



T



U: CM 1
YIELD 90%

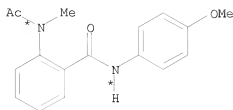


U: CM 2
YIELD 90%

RX(10) RCT T 66860-40-0
 RGT C 7601-90-3 HC104
 PRO U 66860-59-1

10/ 562,112

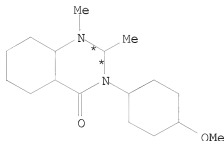
RX(11) OF 11 V ==> W



V



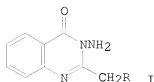
W: CM 1
YIELD 85%



W: CM 2
YIELD 85%

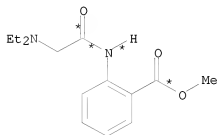
RX(11) RCT V 66860-41-1
RGT C 7601-90-3 HClO4
PRO W 66860-61-5

L3 ANSWER 244 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 87:201459 CASREACT
TITLE: New 3-aminoquinazolinones
AUTHOR(S): Sauter, Fritz; Stanetty, Peter; Jordis, Ulrich
CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Wien, Vienna, Austria
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1977),
310(8), 680-2
CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

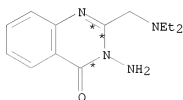


AB Aminoquinazolinones I (R = Net_2 , piperidino, 2,6-dimethylpiperidino, morpholino, 4-methyl-1-piperazinyl) were obtained in 47-98% yield by treating 2-MeO $2\text{CC}_6\text{H}_4\text{NHCCH}_2\text{R}$ (II: R as above) with N_2H_4 . II (R = amino) were obtained by chloroacetylating Me anthranilate, iodinating II (R = Cl), and aminating II (R = I).

RX(1) OF 15 ...A ==> B



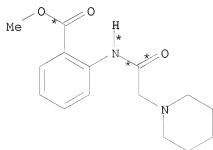
A



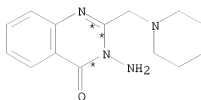
B
YIELD 98%

RX(1) RCT A 64689-29-8
RGT C 302-01-2 N_2H_4
PRO B 64689-30-1

RX(7) OF 15 ...G ==> N



G



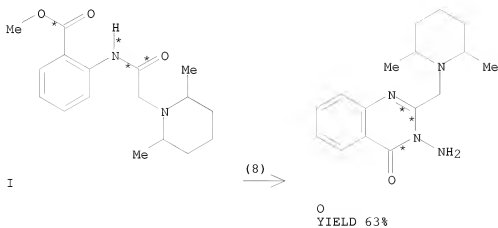
N
YIELD 94%

RX(7) RCT G 64689-25-4

10/ 562,112

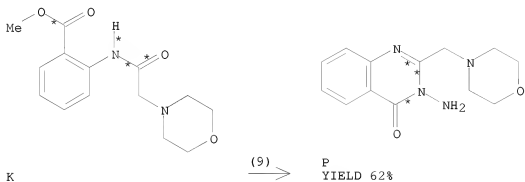
RGT C 302-01-2 N2H4
PRO N 64689-31-2

RX(8) OF 15 ...I ==> O



RX(8) RCT I 64689-26-5
RGT C 302-01-2 N2H4
PRO O 64689-32-3

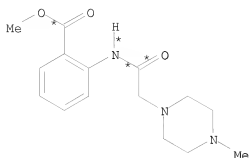
RX(9) OF 15 ...K ==> P



RX(9) RCT K 64689-27-6
RGT C 302-01-2 N2H4
PRO P 64689-33-4

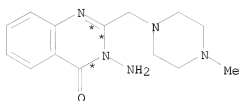
RX(10) OF 15 ...M ==> Q

10/ 562,112



M

(10)

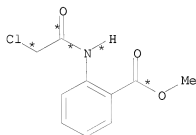


Q

YIELD 47%

RX(10) RCT M 342414-65-7
RGT C 302-01-2 N2H4
PRO Q 64689-34-5

RX(11) OF 15 COMPOSED OF RX(2), RX(1)
RX(11) D + E ==> B



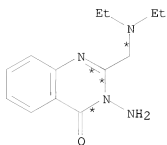
D



E

2
STEPS

10/ 562,112

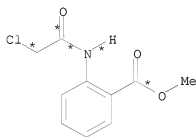


B
YIELD 98%

RX(2) RCT D 58915-18-7, E 109-89-7
PRO A 64689-29-8

RX(1) RCT A 64689-29-8
RGT C 302-01-2 N2H4
PRO B 64689-30-1

RX(12) OF 15 COMPOSED OF RX(3), RX(7)
RX(12) D + F ==> N

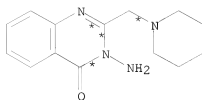


D



F

2
STEPS
→



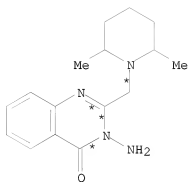
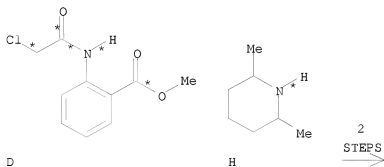
N
YIELD 94%

RX(3) RCT D 58915-18-7, F 110-89-4
PRO G 64689-25-4

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RX(7) RCT G 64689-25-4
 RGT C 302-01-2 N2H4
 PRO N 64689-31-2

RX(13) OF 15 COMPOSED OF RX(4), RX(8)
 RX(13) D + H ==> O

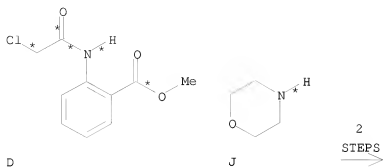


O
 YIELD 63%

RX(4) RCT D 58915-18-7, H 504-03-0
 PRO I 64689-26-5

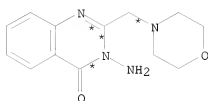
RX(8) RCT I 64689-26-5
 RGT C 302-01-2 N2H4
 PRO O 64689-32-3

RX(14) OF 15 COMPOSED OF RX(5), RX(9)
 RX(14) D + J ==> P



D

J



P

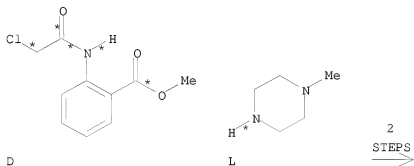
YIELD 62%

RX(5) RCT D 58915-18-7, J 110-91-8
 PRO K 64689-27-6

RX(9) RCT K 64689-27-6
 RGT C 302-01-2 N2H4
 PRO P 64689-33-4

RX(15) OF 15 COMPOSED OF RX(6), RX(10)

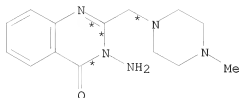
RX(15) D + L ==> Q



D

L

10/ 562,112

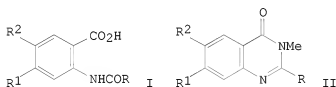


Q
YIELD 47%

RX(6) RCT D 58915-18-7, L 109-01-3
PRO M 342414-65-7

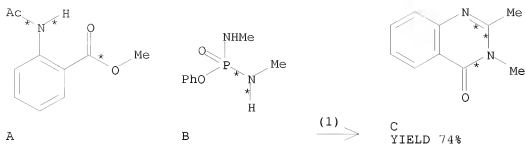
RX(10) RCT M 342414-65-7
RGT C 302-01-2 N2H4
PRO Q 64689-34-5

L3 ANSWER 245 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 87:39404 CASREACT
TITLE: Phosphoramides; III. Phenyl
N,N'-dimethylphosphorodiamidate as a new reagent for
the synthesis of
3-methyl-4-oxo-3,4-dihydroquinazolines
Pedersen, E. B.
AUTHOR(S): Dep. Chem., Odense Univ., Odense, Den.
CORPORATE SOURCE: Synthesis (1977), (3), 180-1
SOURCE: CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



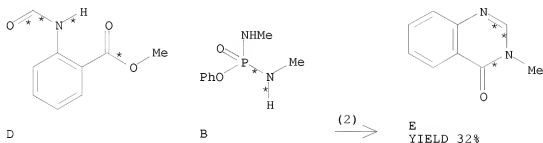
AB Treatment of the acylanthranilates I (R = H, Me, Et, Ph; R1, R2 = H, Me, MeO) with PhOP(O)(NHMe)2 at 250° gave the quinazolinones II in 32-74% yields.

RX(1) OF 6 A + B ==> C



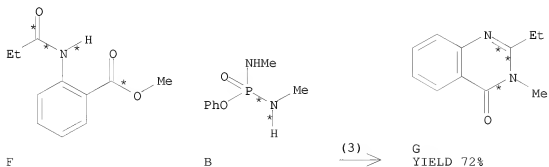
RX(1) RCT A 2719-08-6, B 1754-58-1
 PRO C 1769-25-1

RX(2) OF 6 D + B \implies E



RX(2) RCT D 41270-80-8, B 1754-58-1
 PRO E 2436-66-0

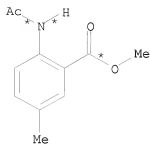
RX(3) OF 6 F + B \implies G



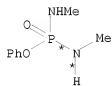
RX(3) RCT F 25628-84-6, B 1754-58-1
 PRO G 58718-53-9

10/ 562,112

RX(5) OF 6 J + B ==> K

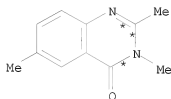


J



B

(5) 



K

YIELD 40%

RX(5) RCT J 37619-22-0, B 1754-58-1
PRO K 63190-58-9

L3 ANSWER 246 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 85,123848 CASREACT

TITLE: Synthesis and chemotherapeutic study of substituted 2-styryl-4-amino-6-methoxyquinazolines

AUTHOR(S): Zhikhareva, G. P.; Pronina, E. V.; Golovanova, E. A.; Pershin, G. N.; Novitskaya, N. A.; Zykova, T. N.; Gus'kova, T. A.; Yakhontov, L. N.

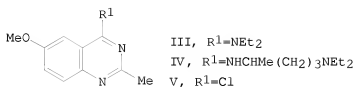
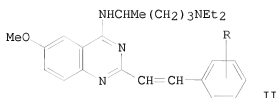
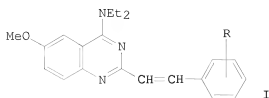
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1976), 10(4), 62-6
CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal

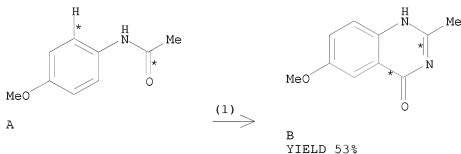
LANGUAGE: Russian

GI



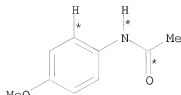
AB The quinazolines I and II (R = o-Cl, p-Cl, p-Br, o-NO₂, p-NO₂) were prepared in 18-65% yield by condensation of III and IV, resp., with RC₆H₄CHO. III and IV were prepared by reaction of p-MeOC₆H₄NHAc with H₂NCO₂Et to give 53% 6-methoxy-2-methyl-4-quinazolone; this was converted to V, which was treated with Et₂NH and H₂NCHMe(CH₂)₃NEt₂, resp. II (R = o-Cl) has min. inhibitory concentration of 4-30 µg/ml against gram-pos. bacteria; I (R = o-Cl) and II (R = o-Cl, o-NO₂) have min. inhibitory concns. of 0.5-8 µg/ml against tuberculosis mycobacteria. The growth of fungi was inhibited only at high concns.

RX(1) OF 9 A ==> B...



RX(1) RCT A 51-66-1
 PRO B 51413-71-9

RX(9) OF 9 COMPOSED OF RX(1), RX(2), RX(4)
RX(9) A + G ==> H

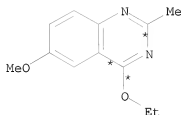


A



G

3
STEPS
→



● HCl

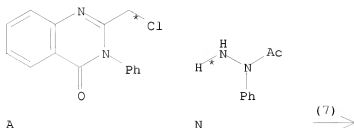
H

YIELD 82%

RX(1)	RCT	A 51-66-1
	PRO	B 51413-71-9
RX(2)	RCT	B 51413-71-9
	RGT	D 10025-87-3 POC13
	PRO	C 60395-90-6
RX(4)	RCT	C 60395-90-6, G 64-17-5
	PRO	H 60395-91-7
	SOL	64-17-5 EtOH

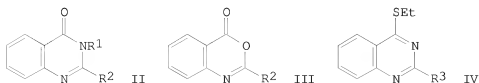
L3 ANSWER 247 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 85:46575 CASREACT
 TITLE: Studies on 4-quinazolinone. IV. Synthesis and properties of 2-(β-phenylhydrazinomethyl)-3-aryl-4-quinazolinones
 Kozhevnikov, Yu. V.
 AUTHOR(S): Nauch. Tr. Perm. Farmatsevt. In-t (1975), (8), 35-7
 CORPORATE SOURCE: USSR
 SOURCE: From: Ref. Zh., Khim. 1976, Abstr. No. 9Zh276
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 AB Title only translated.

RX(7) OF 11 A + N ==> O



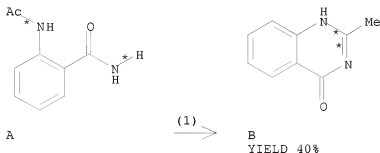
RX(7) RCT A 22312-77-2, N 2116-41-8
 PRO O 60431-83-6

L3 ANSWER 248 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 85:21282 CASREACT
 TITLE: Reaction of triethyloxonium fluoroborate with acid
 amide. III. Formation of quinazoline and
 4H-3,1-benzoxazin-4-one derivatives
 AUTHOR(S): Kato, Takehiko; Takada, Atsushi; Ueda, Takeo
 CORPORATE SOURCE: Sch. Pharm. Sci., Kitasato Univ., Tokyo, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1976), 24(3),
 431-6
 CODEN: CPBIAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



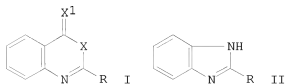
AB Reaction of o-R1NHCO C6H4NHCOR2 (I, R1 = H, Me, Et, Pr, Ph, o-C6H4Me, -C6H4OMe, -C6H4OEt, CH2Ph; R2 = Me, Et, Pr, CHMe2) with Et3O+BF4- gave the quinazolinones II, whereas I (R1 = H, R2 = Ph, o-, p-tolyl, p-C6H4OMe, o-, p-C6H4Cl) gave the quinoxazinones III and o-H2NC(S)C6H4NHCOR3 (R3 = Ph, Me, Et, p-C6H4R4, R4 = Me, OMe, Cl, NO2), the quinazolines IV.

RX(1) OF 1 A ==> B



RX(1) RCT A 33809-77-7
RGT C 368-39-8 Et3O.BF4
PRO B 1769-24-0
SOL 75-09-2 CH2Cl2
NTE Classification: Condensation; Heterocycle formation;
Cyclisation; Isomerisation; # Conditions: Et3O.BF4 CH2Cl2; Rf 1h

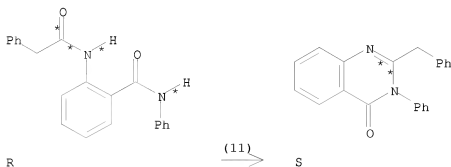
L3 ANSWER 249 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 84:135575 CASREACT
TITLE: Condensation reactions between o-phenylenediamine and
2-substituted 1,3-benzoxazin-4-ones
AUTHOR(S): Rabilloud, Guy; Sillion, Bernard
CORPORATE SOURCE: Inst. Fr. Pet., CEN, Grenoble, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1975),
(11-12, Pt. 2), 2682-6
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
GI



AB Condensation of benzoxazinones I (X = X1 = O, R = Me, CH2Ph, Ph, Bz) with

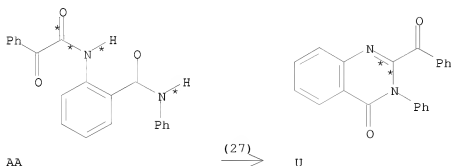
o-(H2N)2C6H4 gave the benzimidazoles II (R = Me, CH2Ph, Ph, 2-PhCH2COC6H4), I (XX1 = o-NC6H4N:, R = CH2Ph, Ph), I (X1 = O, XR = o-NC6H4N:CPh) and 2-(2-H2NC6H4NHCO)C6H4NHBz. Reaction of I (X = X1 = O, R = CH2Ph, Bz) with PhNH2 gave I (X = NPh, X1 = O).

RX(11) OF 73 ...R ==> S...



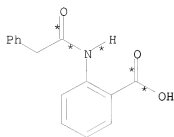
RX(11) RCT R 74772-50-2
 PRO S 19857-34-2
 CAT 108-39-4 3-Methylphenol

RX(27) OF 73 ...AA ==> U



RX(27) RCT AA 341545-11-7
 PRO U 58980-14-6
 CAT 108-39-4 3-Methylphenol

RX(33) OF 73 COMPOSED OF RX(9), RX(12)
 RX(33) N + T ==> S

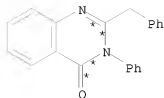


N



T

2
STEPS
→

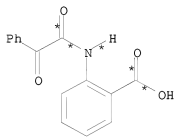


S

RX(9) RCT N 28565-98-2
PRO J 58980-13-5
CAT 108-24-7 Ac2O

RX(12) RCT J 58980-13-5, T 62-53-3
PRO S 19857-34-2
CAT 108-39-4 3-Methylphenol

RX(40) OF 73 COMPOSED OF RX(26), RX(14)
RX(40) AB + T ==> U

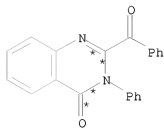


AB



T

2
STEPS
→

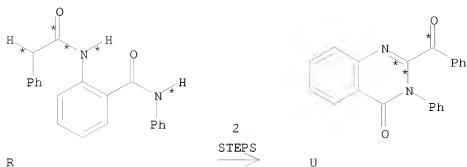


U

RX(26) RCT AB 58980-12-4
PRO P 28565-99-3
CAT 108-24-7 Ac2O

RX(14) RCT P 28565-99-3, T 62-53-3
PRO U 58980-14-6
CAT 108-39-4 3-Methylphenol

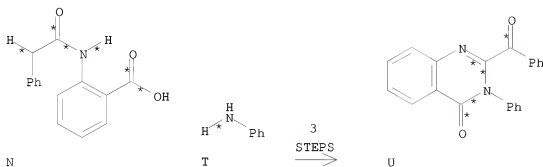
RX(43) OF 73 COMPOSED OF RX(11), RX(13)
RX(43) R ==> U



RX(11) RCT R 74772-50-2
 PRO S 19857-34-2
 CAT 108-39-4 3-Methylphenol

RX(13) RCT S 19857-34-2
 RGT Q 7446-08-4 SeO2
 PRO U 58980-14-6
 CAT 108-24-7 Ac2O

RX(55) OF 73 COMPOSED OF RX(9), RX(10), RX(14)
 RX(55) N + T ==> U

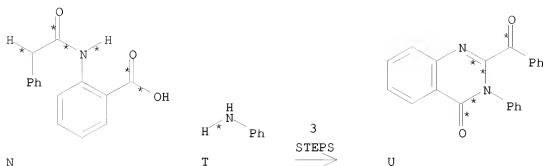


RX(9) RCT N 28565-98-2
 PRO J 58980-13-5
 CAT 108-24-7 Ac2O

RX(10) RCT J 58980-13-5
 RGT Q 7446-08-4 SeO2
 PRO P 28565-99-3
 CAT 108-24-7 Ac2O

RX(14) RCT P 28565-99-3, T 62-53-3
 PRO U 58980-14-6
 CAT 108-39-4 3-Methylphenol

RX(58) OF 73 COMPOSED OF RX(9), RX(12), RX(13)
 RX(58) N + T ==> U



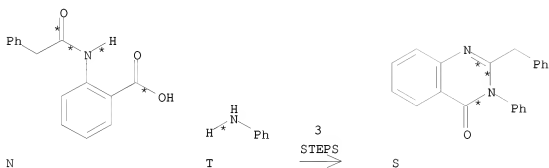
RX(9) RCT N 28565-98-2
 PRO J 58980-13-5
 CAT 108-24-7 Ac2O

RX(12) RCT J 58980-13-5, T 62-53-3
 PRO S 19857-34-2
 CAT 108-39-4 3-Methylphenol

RX(13) RCT S 19857-34-2
 RGT Q 7446-08-4 SeO2
 PRO U 58980-14-6
 CAT 108-24-7 Ac2O

RX(60) OF 73 COMPOSED OF RX(9), RX(22), RX(11)

RX(60) N + T ==> S



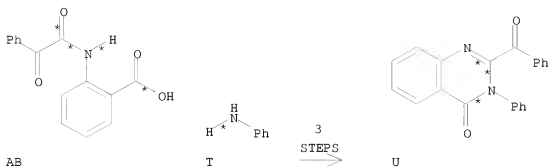
RX(9) RCT N 28565-98-2
 PRO J 58980-13-5
 CAT 108-24-7 Ac2O

RX(22) RCT J 58980-13-5, T 62-53-3
 PRO R 74772-50-2
 CAT 108-39-4 3-Methylphenol

RX(11) RCT R 74772-50-2
 PRO S 19857-34-2
 CAT 108-39-4 3-Methylphenol

RX(68) OF 73 COMPOSED OF RX(26), RX(23), RX(27)

RX(68) AB + T ==> U



RX(26) RCT AB 58980-12-4

PRO P 28565-99-3

CAT 108-24-7 Ac2O

RX(23) RCT P 28565-99-3, T 62-53-3

PRO AA 341545-11-7

CAT 108-39-4 3-Methylphenol

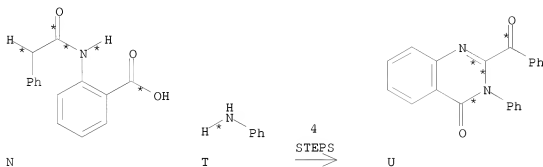
RX(27) RCT AA 341545-11-7

PRO U 58980-14-6

CAT 108-39-4 3-Methylphenol

RX(69) OF 73 COMPOSED OF RX(9), RX(10), RX(23), RX(27)

RX(69) N + T ==> U



RX(9) RCT N 28565-98-2

PRO J 58980-13-5

CAT 108-24-7 Ac2O

RX(10) RCT J 58980-13-5

RGT Q 7446-08-4 SeO2

PRO P 28565-99-3

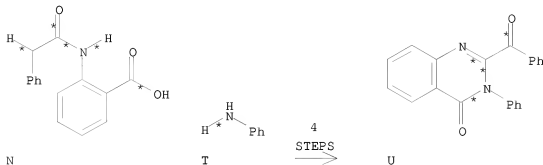
CAT 108-24-7 Ac2O

RX(23) RCT P 28565-99-3, T 62-53-3

PRO AA 341545-11-7
 CAT 108-39-4 3-Methylphenol

RX(27) RCT AA 341545-11-7
 PRO U 58980-14-6
 CAT 108-39-4 3-Methylphenol

RX(71) OF 73 COMPOSED OF RX(9), RX(22), RX(11), RX(13)
 RX(71) N + T ==> U



RX(9) RCT N 28565-98-2
 PRO J 58980-13-5
 CAT 108-24-7 Ac2O

RX(22) RCT J 58980-13-5, T 62-53-3
 PRO R 74772-50-2
 CAT 108-39-4 3-Methylphenol

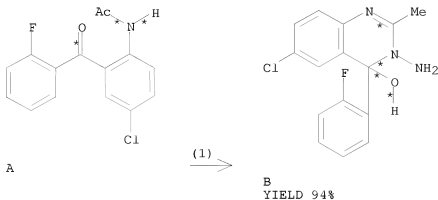
RX(11) RCT R 74772-50-2
 PRO S 19857-34-2
 CAT 108-39-4 3-Methylphenol

RX(13) RCT S 19857-34-2
 RGT Q 7446-08-4 SeO2
 PRO U 58980-14-6
 CAT 108-24-7 Ac2O

L3 ANSWER 250 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 83:193188 CASREACT
 TITLE: Quinazolines and 1,4-benzodiazepines. LXXI.
 Reactions of 2-(triazol-4-yl)benzophenones
 AUTHOR(S): Walser, Armin; Flynn, Thomas; Fryer, R. Ian
 CORPORATE SOURCE: Res. Div., Hoffmann-La Roche, Inc., Nutley, NJ, USA
 SOURCE: Journal of Heterocyclic Chemistry (1975), 12(4),
 717-24
 CODEN: JHTCAD; ISSN: 0022-152X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Some new triazolylbenzophenones, e.g. I (R = H), were prepared by reaction

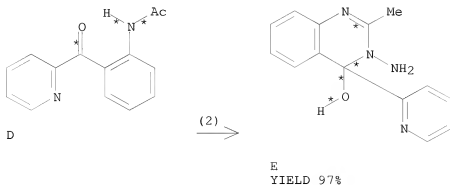
of the corresponding quinazolines, e.g. II, with HCO_2H . The triazolylbenzophenones were converted to triazolobenzodiazepines, e.g. III. The reaction of I ($\text{R} = \text{CHO}$) with hydrazine yielded the triazoloquinolines IV and V. The cyclization of the benzophenones, e.g. I ($\text{R} = \text{H}$), gave triazoloindoles, e.g. VI ($\text{R} = \text{H}$), which were alkylated to derivs. with basic and acidic side chains. Quaternization of compound VI ($\text{R} = \text{CH}_2\text{CO}_2\text{Et}$) with $\text{BrCH}_2\text{CO}_2\text{Et}$ followed by treatment with hydroxide resulted in the formation of the triazinoindole V.

RX(1) OF 49 A ==> B...



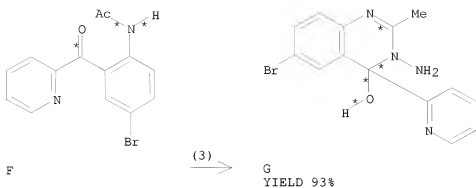
RX(1) RCT A 57698-59-6
 RGT C 302-01-2 N2H4
 PRO B 57698-27-8

RX(2) OF 49 D ==> E...



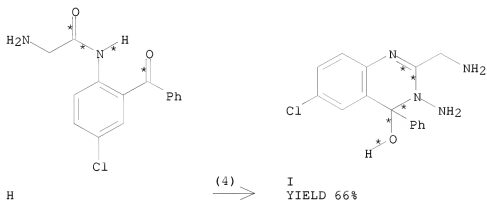
RX(2) RCT D 1770-89-4
 RGT C 302-01-2 N2H4
 PRO E 57698-28-9

RX(3) OF 49 F ==> G...



RX(3) RCT F 1770-90-7
 RGT C 302-01-2 N2H4
 PRO G 57698-29-0

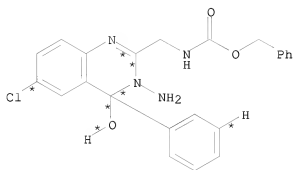
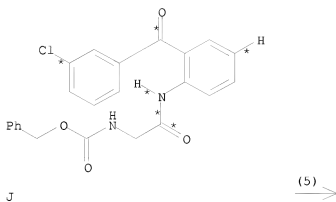
RX(4) OF 49 H ==> I



RX(4) RCT H 5504-71-2
 RGT C 302-01-2 N2H4
 PRO I 57698-31-4

RX(5) OF 49 J ==> K...

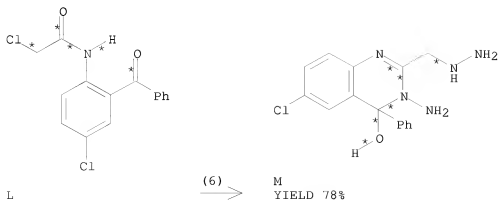
10/ 562,112



K
YIELD 67%

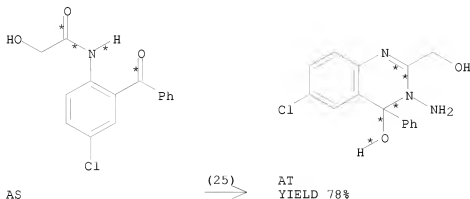
RX(5) RCT J 340171-33-7
 RGT C 302-01-2 N2H4
 PRO K 57698-32-5

RX(6) OF 49 L ==> M



RX(6) RCT L 4016-85-7
 RGT C 302-01-2 N2H4
 PRO M 57698-33-6

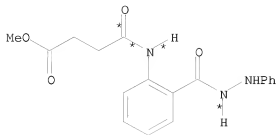
RX(25) OF 49 AS ==> AT...



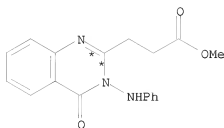
RX(25) RCT AS 5628-03-5
 RGT C 302-01-2 N2H4
 PRO AT 57698-30-3

L3 ANSWER 251 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 83:28178 CASREACT
 TITLE: 4-Quinazolinone series. VI. Synthesis and properties of 2-(β -carbomethoxyethyl)-3-arylamino-substituted 4-quinazolinone
 AUTHOR(S): Kozhevnikov, Yu. V.
 CORPORATE SOURCE: Perm. Farm. Inst., Perm, USSR
 SOURCE: Izvestiya Vysshikh Uchebnykh Zavedenii, Khimiya i Khimicheskaya Tekhnologiya (1975), 18(2), 235-7
 CODEN: IVUKAR; ISSN: 0579-2991
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI For diagram(s), see printed CA Issue.
 AB 4-Quinazolinones (I; R = H, o-, m-, p-Me, o-, m-, p-Cl, o-, m-, p-Br, 4-bromo-2-methyl) were prepared in 30-88% yields by reaction of benzoxazinepropionate (II) with RC6H4NHNH2 in PhMe containing PC13.

RX(1) OF 14 ...A ==> B



A



B

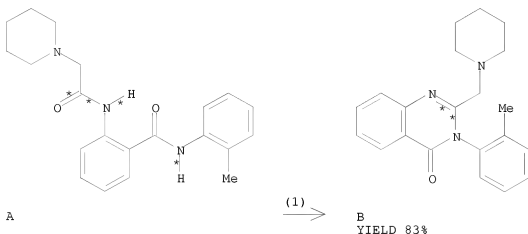
YIELD 31%

RX(1) RCT A 56056-26-9
 RGT C 7719-12-2 PC13
 PRO B 56056-14-5

L3 ANSWER 252 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 69:96650 CASREACT
 TITLE: 2-Dialkylaminomethyl- and
 2-[β-(dialkylamino)ethyl]-3-aryl-4-oxo-3,4-
 dihydroquinazoline
 AUTHOR(S): Pesson, Marcel; Richer, Denise
 CORPORATE SOURCE: Lab. Roger Bellon, Neuilly-sur-Seine, Fr.
 SOURCE: Comptes Rendus des Seances de l'Academie des Sciences,
 Serie C: Sciences Chimiques (1968), 266(26), 1787-90
 CODEN: CHDCAQ; ISSN: 0567-6541
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 GI For diagram(s), see printed CA Issue.
 AB I, where n is 1 or 2 and R is piperidino, are prepared Thus,
 o-H2NC6H4CONHC6H4Me-o is treated with ClCH2COC1 in a NaOAcHOAc mixture to
 give 69% o-ClCH2CONHC6H4CONHC6H4Me-o (II), m. 180°. Similarly
 prepared are o-ClCH2CONHC6H4CONHPh, m. 190°, and
 o-ClCH2CH2CONHC6H4CONHC6H4Me-o, m. 173°. A mixture of II,
 piperidine, and C6H6 is refluxed to give o-(piperidinoacetamido)benzoic
 acid o-toluidide (III), m. 163°. Similarly prepared are

o-(piperidinoacetamido)benzanilide, m. 176°, and o-(β-piperidinopropionamido)benzoic acid o-toluidide, m. 114-15°. A mixture of III and HOAc is refluxed 6 hrs. to give 83% 2-(piperidinomethyl)-3-(o-tolyl)-4-oxo-3,4-dihydroquinazoline (IV), m. 88-9°. Similarly prepared are I (n = 1, R = piperidino, Ar = Ph), m. 128°, and I (n = 2, R = piperidino, Ar = o-tolyl) (V) (prepared in anisole), 121°. Uv and ir data for IV and V and N.M.R. data for IV are given. A mixture of III and Ac2O is heated to give o-AcNHC6H4CO2H (m. 192°) and N,N-pentamethyleneglycine o-toluidide (m. 96-8°). A mixture of II in HOAc is refluxed to give I (n = 1, R = Cl, Ar = o-tolyl) (VI), m. 108-10°, which is hydrogenated (5% Pd/C) to give I (n = 1, R = H, Ar = o-tolyl), m. 115°. A mixture of VI, piperidine, and C6H6 is refluxed to give IV, m. 88-90°.

RX(1) OF 1 A ==> B



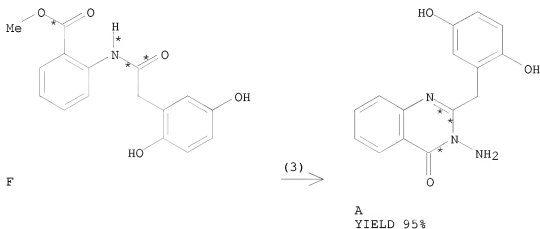
RX(1) RCT A 19806-75-8
 RGT C 64-19-7 AcOH
 PRO B 19806-76-9
 NTE Classification: Condensation; Heterocycle formation;
 Cyclisation; # Conditions: AcOH heat 6h

L3 ANSWER 253 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 66:18698 CASREACT
 TITLE: Preparation and properties of some substituted
 quiazolino[3,2-b]cinolines
 AUTHOR(S): Kort, M. J.; Lamchen, Max
 CORPORATE SOURCE: Univ. Cape Town, Cape Town, S. Afr.
 SOURCE: Journal of the Chemical Society [Section] C: Organic
 (1966), (23), 2190-6
 CODEN: JSOAX; ISSN: 0022-4952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB The preps. of the substituted quiazolino

3-amino-2-(2,5-dihydroxybenzyl)quinazolin-4(3H)-one (I) and some of its derivs. are described. When this quinol is oxidized with an acidic ferric chloride solution or with an aqueous sodium hydroxide solution a quinone was formed,

but it spontaneously ring-closed to give quinazolino[3,2-b]cinnoline-2,7(13H)-dione (II), which was isolated as the hydrochloride. When the oxidation of the quinol was carried out with an acidic hydrogen peroxide solution the ring-closed product also formed as an intermediate, which was immediately converted into 1,3,4-trichloroquinazoline[3,2-b]-cinnoline-2,7(13H)-dione, and only this dione was then obtained.

RX(3) OF 6 ...F ==> A...



RX(3) RCT F 13162-86-2
 RGT G 302-01-2 N2H4
 PRO A 13162-88-4
 SOL 7732-18-5 Water, 64-17-5 EtOH
 NTE Classification: Annellation; Condensation; Hydrazination;
 Heterocycle formation; # Conditions: N2H4 H2O EtOH; Rf 3h

L3 ANSWER 254 OF 258 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 55:13443 CASREACT

TITLE: 2,3-Disubstituted 3H-4-quinazolones and
 3H-4-thioquinazolones

AUTHOR(S): Jackman, G. B.; Petrow, V.; Stephenson, O.
 SOURCE: Journal of Pharmacy and Pharmacology (1960), 12,
 529-38

CODEN: JPPMAB; ISSN: 0022-3573

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Typical procedures in the synthesis of some
 2-alkyl-3-aryl-3H-4-quinazolones and conversion to thio derivs. follow. A
 solution of 8 ml. PCl3 in 50 ml. PhMe was added to a stirred mixture of 34.4 g.
 p-bromoaniline (I) and acetylanthranilic acid (II) at room temperature, the
 resulting paste was refluxed 2 hrs., cooled, 15% Na2CO3 solution added, and

the PhMe steam-distilled to give 27 g.

3-p-bromophenyl-2-methyl-3H-4-quinazolone (III), which was crystallized from 95% EtOH; HCl salt (IV) m. approx. 260° (decomposition) (95% EtOH).

Addition of 11.4 g. dicyclohexylcarbodiimide in 50 ml. tetrahydrofuran (THF) to 8.9 g. I and 9 g. II in 100 ml. THF and, after 5 hrs. at room temperature, addition of 1.5 ml. AcOH, precipitated dicyclohexylurea, which was filtered off after 2 hrs. Evaporation of the filtrate to dryness in vacuo, dissoln. of the residue in 150 ml. EtOAc and shaking with 2N HCl precipitated 9 g. IV; and washing the filtered EtOAc solution with 1N Na2CO3 and H2O, then concentrating

to 50

ml. gave 1.5 g. 2-acetamido-4'-bromobenzanilide, m. 215-16°.

PhSO2Cl (17.8 g.) was added to 17.9 g. II in 30 ml. C5H5N then 16.2 g.

2,4-dichloroaniline was added portionwise, the mixture heated 2 hrs. over steam, cooled, and diluted with H2O to give

3-(2,4-dichlorophenyl)-2-methyl-3H-quinazolone as a gum which solidified on trituration with EtOH and yielded 9.6 g. needles, m. 151-2°

(EtOAc-petr. ether); HCl salt m. 242-50° (MeOH). A mixture of II and 2,4-dichloroaniline in C5H5N with PCl3 added dropwise gave the above

product, separated as the HCl salt, m. 240-50°. Prepared as intermediates were (m.p. given): 4-bromo-2,3-dimethylacetanilide,

158-60° (long needles, aqueous-EtOH) [HCl salt, m. 268° (decomposition), with NaOH and steam distillation gave

4-bromo-2,3-dimethylaniline,

m. 32-4° (plates, petr. ether)];

4-bromo-2,3-dimethyl-6-nitroacetanilide, 207-9° (pale yellow needles, 95% EtOH); 4-bromo-2,3-dimethyl-6-nitroaniline, 147-9°

(flat golden-brown needles, 50% EtOH);

5-bromo-3,4-dimethyl-o-phenylenediamine, 85-7° (petr. ether). The following 2-alkyl-3-aryl-3H-4-quinazolones were prepared (alkyl and aryl

substituents, resp., base or HCl salt, indicated by B or H, resp., and m.p. given; all the HCl salts melted with decomposition over a range of several

degrees): Me, p-anisyl, H 240°; Me, o-phenetyl, B 115-16°, H 215°; Me, m-phenetyl, B 130-2°, H 225°; Me,

p-phenetyl, H 240°; Me, 3,4,5-trimethoxyphenyl, B 150-2°, H 250°; Me, 2,3-xylyl, B 172-3°, H 240°; Me, 2,4-xylyl,

B 100-2°, H 240°; Me, 2,5-xylyl, B 125-7°; Me,

2,6-xylyl, H 215°; Me, 3,4-xylyl, B 134-6°; Me, p-FC6H4, B

133-4°, H 280°; Me, o-ClC6H4, B 130-2°; Et, o-ClC6H4,

B 124-6°; Me, m-ClC6H4, B 133-5°; Me, o-BrC6H4, B

147-8°, H 220°; Me, m-BrC6H4, B 134-6°, H

260°; Me, p-BrC6H4, B 170-2°, H 260°; Et, p-BrC6H4, B

170-2°; Pr, p-BrC6H4, B 139-41°; Me, p-IC6H4, B

178-80°, H 265°; Me, 2,4-ClC6H3, B 151-2°, H

250°; Me, 2,5-ClC6H3, B 161-3°, H 244°; Me,

4-bromo-2,3-xylyl, B 168-70°. Thioquinazolone derivs. were prepared

by refluxing the quinazolone with P2S5 in xylene, cooling, adding NaOH and distilling with steam. 2-Alkyl-3-aryl-3H-4-thioquinazolones prepared were

(alkyl, aryl, base or HCl salt, and m.p. given, resp.): Me, o-tolyl, B

121-3°, H 228-30°; Me, p-FC6H4, B 128-30°; Me,

p-ClC6H4, B 183-5°; Me, o-BrC6H4, B 174-6°; Me, p-BrC6H4, B

190-2°; Et, p-BrC6H4, B 168-70°.

N-Alkyl-2-benzamidobenzamides prepared were (alkyl at -CONHR, aryl at -NHCOAr, and m.p., resp.): H, p-BrC6H4, 224-6°; Me, o-tolyl,

167-70°; Me, p-ClC6H4, 162-4° and 190-2°; Me,

o-BrC6H4, 170-2°; Me, p-BrC6H4, 165° and 197-9°; Et,

Ph, 158-60°; Et, p-BrC6H4, 174-6°; Bu, Ph, 125-7°.

3-Methyl-2-o-tolyl-3H-4-quinazolone was prepared by refluxing 26.7 g.

N-methyl-2-(o-methylbenzamido)benzamide with 300 ml. 5% NaOH containing 50 ml.

EtOH, and also from 4 g. 2-o-tolyl-3H-4-quinazolone in 80 ml. 1N NaOH and

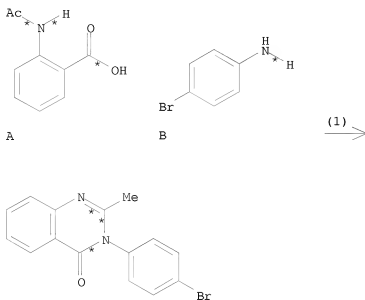
Me2SO4 (dropwise). The products (56% and 50%, resp.) were purified by

crystallization from petr. ether and aqueous EtOH. The HCl salt crystallized from EtOH.

The 3-alkyl-2-aryl-3H-4-quinazolones prepared were (alkyl, aryl, base or HCl salt, and m.p., resp., given): Me, Ph, B 136-8°, H 208° (decomposition); Et, Ph, B 130-2°, H 205° (decomposition); Bu, Ph, B 116-18°; 2,3-dihydroxypropyl, Ph, B 179-81°; Me, o-tolyl, B 107-9°, H 205° (decomposition); Me, p-ClC₆H₄, B 170-2°; Me, o-BrC₆H₄, B 154-6°; H, p-BrC₆H₄, B 313-5°; Me, p-BrC₆H₄, B 170-2°; Et, p-BrC₆H₄, 122-4°, 138-40°.

2-p-Bromophenyl-3-methyl-3H-4-quinazolinone (44.1 g.) in 400 ml. xylene was refluxed 2 hrs. with 37.4 g. P2S5, 275 ml. 10% NaOH was added cautiously to the cooled mixture, and the xylene steam-distilled to give 42 g. 2-p-bromophenyl-3-methyl-3H-4-thioquinazolinone, m. 167-9°, yellow hair-like crystals from 2 l. EtOH.

RX(1) OF 1 A + B ==> C



C
YIELD 45%

RX(1) RCT A 89-52-1, B 106-40-1
 PRO C 1788-95-0
 SOL 108-88-3 PhMe
 NTE Classification: Heterocycle formation; C-Amination;
 Condensation; # Conditions: PCl₃ toluene; 20 deg; Rf 2h

L3 ANSWER 255 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 52:50665 CASREACT
 TITLE: Research in the 2-methyl-3-aryl-4-quinazolinone series
 AUTHOR(S): Serventi, Giorgio; Marchesi, Renato
 CORPORATE SOURCE: Univ. Parma, Italy

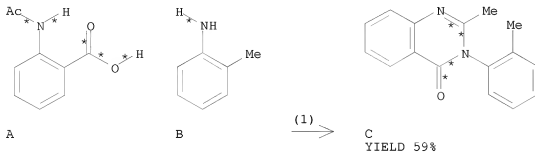
SOURCE: Bollettino Scientifico della Facolta di Chimica Industriale di Bologna (1957), 15, 117-20
 CODEN: BSFCAY; ISSN: 0366-3205

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB This series was studied for its promise of yielding antimalarial and analgesic agents. PC13 (0.033 mole) in 20 cc. PhMe added dropwise to 0.1 mole acetylanthranilic acid and 0.1 mole arylamine in 200 cc. PhMe, the mixture refluxed 2 hrs. and made alkaline with aqueous Na2CO3 (10%), and the solid recrystd. several times gave 2-methyl-3-aryl-4-quinazolones (3-aryl group, m.p., and % yield given): Ph, 146-7°, 86; o-tolyl (o-I), 120°, 59; m-I, 129°, 51; p-I, 149-50°, 68; o-chlorophenyl (o-II), 120°, 43; m-II, 130°, 63.19; p-II, 157°, 80; o-anisyl (o-III), 132°, 55.3; m-III, 152°, 72; p-III, 170°, 70; o-carbomethoxyphenyl (o-IV), 120°, 53.2; m-IV, 132°, 48; p-IV, 198°, 65.3. 2-Methyl-3-(o-carboxyphenyl)-4-quinazolone was prepared by treating 0.1 mole I with 0.15 mole NaOH in 50 cc. EtOH (50%), refluxing 4 hrs., acidifying, and crystallizing from AcOH, m. 246-7°, yield 33%; the m-isomer m. 276°, yield 42.5%; p-isomer, m. 281°, yield 39.5%. A table of ultraviolet spectral data at three wavelengths is also given.

RX(1) OF 1 A + B ==> C



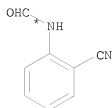
RX(1) RCT A 89-52-1, B 95-53-4
 PRO C 72-44-6
 SOL 108-88-3 PhMe
 NTE Classification: Annellation; Heterocycle formation; C-Amination;
 Condensation; # Conditions: PC13 toluene; Rf 2h; # Comments:
 Also C.A., 9147 (1958).

L3 ANSWER 256 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 51:85734 CASREACT
 ACCESSION NUMBER: Preparation of quinazoline derivatives through
 TITLE: ring-closure of aromatic o-cyano(acylamino) compounds
 in alkaline alcoholic or phenolic medium. I.
 4-RO-substituted quinazolines
 AUTHOR(S): Breukink, K. W.; Krol, L. H.; Verkade, P. E.; Wepster,

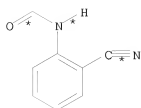
B. M.
 CORPORATE SOURCE: Tech. Univ., Delft, Neth.
 SOURCE: Recueil des Travaux Chimiques des Pays-Bas et de la Belgique (1957), 76, 401-14
 CODEN: RTCPB4; ISSN: 0370-7539
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB On boiling aromatic o-cyano(acylamino) compds. in alkaline alc. or phenolic solution, 4-RO substituted quinazolines are formed. The diazonium salt from the diazotization of o-O2NC6H4NH2 (cf. Fieser and Thompson, C.A. 33, 21211) treated according to Bogert and Hand [J. Am. Chemical Society 24, 1035(1902)] yielded pure o-NCC6H4NO2, m. 109-10°, reduced with SnCl2 and concentrated HCl, and the product purified by distillation in vacuo to give 82% pure o-NCC6H4NH2 (I), b18 138-9°; picrate, m. 108-9° I (6.10 g.) in 75 ml. dry Et2O and 8.5 ml. freshly prepared AcOCHO (cf. Clemo and Swan, C.A. 40, 5811) filtered after 24 hrs. and the crystalline product (7.11 g.) recrystd. from 1:1 C6H6-petr. ether gave 6.92 g. pure o-NCC6H4NHCHO (II), m. 130.5-1.5°. II (5.00 g.) refluxed with 75 ml. 0.05N NaOMe in absolute MeOH with addition of 5, 5, and 10 ml. 0.5N NaOMe in MeOH after 2, 3, and 3.5 hrs., the alkaline solution distilled in vacuo after 4 hrs., the residue extracted with Et2O, the washed and dried extract evaporated, and the residue distilled in vacuo gave 4.83 g. strongly hygroscopic oil, treated with 50 ml. petr. ether 24 hrs. at room temperature to give 1.69 g. I, m. 48-9°. The petr. ether mother liquor filtered and evaporated, the residue taken up in 50 ml. MeOH, treated with 4 g. picric acid in 25 ml. MeOH, and filtered immediately, the precipitate washed with MeOH, dried, and crystd, from PhMe gave 5.31 g. picrate, m. 175.5-6.5°, decomposed with aqueous LiOH and extracted with Et2O to give 4-methoxyquinazoline (III), m. 35-6°, b11 127-8°, strongly hygroscopic. Conversion of the known 4-hydroxyquinazoline (IIIA) according to Endicott, et al. (C.A. 40, 57482), gave 4-chloroquinazoline (IV), m. 97-8°. On completion of the exothermic reaction between 10 g. IV and 100 ml. N NaOMe in MeOH, the mixture was boiled 15 min., the MeOH evaporated in vacuo, and the residue treated with Et2O and H2O, the Et2O extract dried and evaporated, and the residue fractionated in vacuo to give 7.3 g. III, converted to IIIA by boiling in dilute HCl. I (6.00 g.) in 100 ml. dry Et2O kept 24 hrs. at room temperature with 15 ml. Ac2O and filtered gave 7.91 g. o-NCC6H4NHAc (V), m. 133-4° (from Et2O). V (5.00 g.) refluxed in 100 ml. 0.05N NaOMe in MeOH and treated after 2 and 4 hrs. with 5 and 10 ml. 0.5N NaOMe in MeOH, and the solution worked up after 5 hrs. refluxing gave 5.20 g. colorless oil, treated with 40 ml. petr. ether to give 0.30 g. I on filtration after keeping 24 hrs. at room temperature. The petr. ether mother liquor distilled in vacuo, the residue taken up in 50 ml. MeOH, the solution diluted with H2O, cooled to 0°, kept 1 week with further dilution with H2O, and filtered gave 6.05 g. trihydrate, m. 36-7°, dehydrated at 65°/20 mm. to 4-methoxy-2-methylquinazoline, m. 34-5°; picrate, m. 170.0-1.5°. Similarly, refluxing V with NaOEt in EtOH and working up gave 12% I and 82% monohydrate, m. 39.5-40.0°, dehydrated to 4-ethoxy-2-methylquinoline; picrate, m. 178.0-9.5°. V (5.00 g.) heated 20 hrs. at 120° with 0.35 g. Na in 50 ml. dry PhCH2OH, the alc. evaporated in vacuo, the residue suspended in 250 ml. 20% EtOH and filtered, and the crude precipitate crystallized from petr. ether gave 5.47 g. 4-benzoyloxy-2-methylquinazoline, m. 65.5-6.0°; picrate, m.

147.5-8.5°. Similarly, heating 2.50 g. V 20 hrs. with 0.20 g. Na in 25 g. dry pure PhOH at 125°, the PhOH distilled in vacuo, and the residue suspended in 100 ml. 2N NaOH filtered, the precipitate taken up in Et₂O, the washed and dried extract evaporated, the residue taken up in 40 ml. MeOH, treated with C, and filtered, the filtrate diluted with 30 ml. H₂O and heated, and the solution cooled to 0° and filtered gave 3.52 g. monohydrate, m. 71-83°, dehydrated over P₂O₅ in vacuo to 4-phenoxy-2-methylquinazoline, m. 71.0-1.5°. The four 4-RO-2-methylquinazolines gave quant. yields of IIIa on boiling with dilute HCl. I (4.00 g.) and 5.8 g. BzCl in 100 ml. dry Et₂O refluxed 2 hrs. with 4.8 g. anhydrous K₂CO₃, the Et₂O evaporated in vacuo, the residue extracted with H₂O and filtered, and the washed and dried precipitate recrystd. from MeOH gave 5.98 g. o-NCC₆H₄NHPh (VI), m. 159-60°. VI (5.00 g.) refluxed 6 hrs. with 90 ml. 0.1N NaOMe in MeOH, the solvent distilled in vacuo, and Et₂O added to the residue, the washed and dried extract evaporated, and the residue distilled in vacuo gave 0.68 g. I and 3.60 g. fraction, b₃ 189-91°, recrystd. from dilute MeOH to give 3.55 g. 4-methoxy-2-phenylquinazoline, m. 65.5-6.0° (picrate, m. 174.0-5.5°), converted by boiling dilute HCl to 4-hydroxy-2-phenylquinazoline, m. 240-1°. Iodine (100 g.), 50.0 g. p-ClC₆H₄NH₂, 50 g. CaCO₃, 175 ml. Et₂O, and 175 ml. H₂O refluxed 48 hrs. and worked up according to Dains, et al. (C.A. 12, 1646), gave 61.5 g. 4,2-ClC₆H₃NH₂ (VII), m. 40.5-1.5°. The preferential replacement of iodine in VII by a CN group according to Brit. 488,642 (C.A. 33, 4011) gave 4,2-Cl(NC)C₆H₃NH₂ (VIII), m. 95.0-5.5° (from 1:1 petr. ether-C₆H₆). VIII boiled 30 min. with 2N NaOH until evolution of NH₃ ceased, the cold solution neutralized with HCl and saturated NaOAc solution and filtered, and the precipitate crystallized from H₂O in the presence of C gave authentic 5-chloroanthranilic acid, m. 208.5-10.0°, proving the constitution of VIII and VII. VIII (5.00 g.) heated 2 hrs. at 50° in 10 ml. Ac₂O, the mixture poured into 50 ml. H₂O and filtered and the dried precipitate crystallized from 2:1 C₆H₆-petr. ether gave 6.05 g. 4,2-Cl(NC)C₆H₃NHAc (IX), m. 149.5-50.5°. Conversion of IX with no perceptible deacetylation or consumption of the alkaline catalyst rapidly gave 6-chloro-4-methoxy-2-methylquinazoline, m. 79-80° (from petr. ether), b₁₂ 155-6° (picrate, m. 168.0-9.5°), and 6-chloro-4-ethoxy-2-methylquinazoline, m. 98.5-9.5°, b₁₃ 160-1° (picrate, m. 188-9°). CuCN (3.5 g.) and 3.3 ml. dry pyridine treated with 25 g. dry PhNO₂ and 9.60 g. 2-bromo- α -acetophthalide (cf. Hodgson and Hathway, C.A. 38, 20304), stirred 2 hrs. at 180-90°, the cooled mixture diluted with H₂O, steam-distilled, and filtered, the washed precipitate dried and extracted several times with 5 ml. portions of EtOH, and the combined alc. exts. treated with C, cooled, and filtered gave 5.92 g. 2-cyano- α -acetophthalide (X), m. 219.5-20.5°. X (2.50 g.) refluxed 30 hrs. with 75 ml. 0.1N NaOMe in absolute MeOH, the alc. evaporated in vacuo, H₂O added to the residue, the mixture filtered, and the washed and dried precipitate crystallized from MeOH gave 2.14 g. 4-methoxy-2-methylbenzo[h]quinazoline, m. 119-20°.

RX(4) OF 5 2 J + H ==> B + G



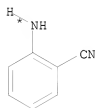
J



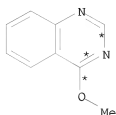
J



H



B



G

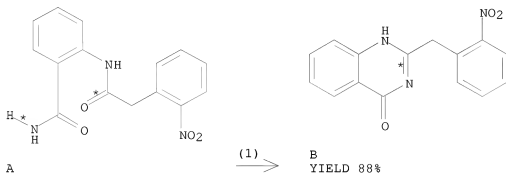
YIELD 42%

RX(4) RCT J 53902-59-3, H 67-56-1
 PRO B 1885-29-6, G 16347-95-8
 SOL 67-56-1 MeOH
 NTE Classification: Deformylation; Heterocycle formation;
 Alkoxylation; # Conditions: MeOH; boil Rf 4h; # Comments: 40%
 yield of ring closure product as picrate; NaOMe used

L3 ANSWER 257 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 42:29858 CASREACT
 ACCESSION NUMBER:
 TITLE: Quinazolines. V. The synthesis of 2- and
 3-(o-aminobenzyl)-4-quinazolones
 AUTHOR(S): Tomisek, A.; Christensen, Bert E.
 CORPORATE SOURCE: Oregon State Coll., Corvallis
 SOURCE: Journal of the American Chemical Society (1948), 70,
 1701-2
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. C.A. 42, 3413b. o-O2NC6H4CH2COC1 (I) (from 5 g. of acid) and 4
 mL. o-H2NC6H4CO2Me in C6H6, gradually treated with 40 mL. 25% KOH,
 give 69% Me N-(o-nitrophenylacetyl)anthranilate (II), m.
 133.5-4° (m.ps. corrected); heated 8 h. at 180° with absolute alc.
 NH3, it gives a good yield of o-O2NC6H4CH2CONH2; the Ac derivative of
 II (not isolated), heated with 14% NH4OH containing a little 10% KOH (1 h. on
 the steam bath), gives 2-methyl-4(3H)-quinazolone, indicating that
 transacylation to o-MeO2CC6H4NHAc had preceded the cyclization. I
 (from 5 g. acid) and 7.6 g. o-H2NC6H4CONH2 in dioxane give 73%
 N-(o-nitrophenyl-acetyl)anthranilamide (III), m. 172-3°;

3.46 g. III, 12 mL. C₅H₅N, 12 mL. H₂O, and 1 mL. 10% NaOH, kept 1 day at room temperature, yield 88% 2-o-nitrobenzyl-4(3H)-quinazoline (IV), m. 254.5° (decomposition). I (from 5 g. acid) and 20 g. o-H₂NC₆H₄CO₂H in dioxane give 82% N-(o-nitrophenyl-acetyl)anthranilic acid (V), m. 224-5° (slow decomposition); 5 g. V and 20 mL. Ac₂O, refluxed 30 min., give 4.4 g. 2-o-nitrobenzyl-4-keto-3,1,4-benzoxazine (VI), m. 165-6°; 5 g. VI in 25 mL. 50% C₅H₅N, saturated with NH₃, allowed to stand 6 h., 1 mL. 10% NaOH added, and the mixture allowed to stand an addnl. 24 h., gives 72% IV. Treatment of 5 g. IV in 300 mL. dilute NaOH with 33 g. FeSO₄·9H₂O in 100 mL. H₂O 7 h. at 80° gives 80% 2-(o-aminobenzyl)-4(3H)-quinazoline, m. above 250° (decomposition); Ac derivative m. 258°. 4-Hydroxy-4(3H)-quinazoline (13 g.), 10 g. o-O₂NC₆H₄CH₂Cl, 5.9 g. 85% KOH, and 200 mL. EtOH, refluxed 6 h., the EtOH removed, and the residue refluxed 15 min. with dilute HCl and C₆H₆, give 3 g. 3-o-nitrobenzyl-4(3H)-quinazoline, m. 169-70°; reduction with SnCl₂ and HCl in AcOH gives 64% 3-(o-aminobenzyl)-4-(3H)-quinazoline, m. 178°.

RX(1) OF 1 A ==> B

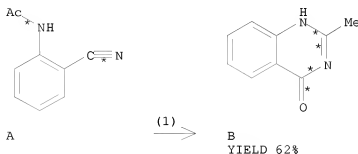


RX(1) RCT A 349135-30-4
 PRO B 7494-72-6
 SOL 7732-18-5 Water, 110-86-1 Pyridine
 NTE Classification: Heterocycle formation; Cyclisation;
 Condensation; Isomerisation; # Conditions: NaOH; H₂O pyridine;
 20 deg 1day

L3 ANSWER 258 OF 258 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 0:406 CASREACT
 TITLE: The synthesis of alkylketodihydroquinazolines from anthranilic nitrile
 AUTHOR(S): Bogert, Marston Taylor; Hand, William Flowers
 CORPORATE SOURCE: Havemeyer Laboratories, Columbia University, USA
 SOURCE: Journal of the American Chemical Society (1902), 24, 1031-1050
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Bogert and Gotthelf have already shown that ketodihydroquinazolines may be

prepared by heating together in sealed tubes anthranilic acid, or its acyl derivatives, with a nitrile, and the reactions there suggested in explanation of this synthesis, taking the case where an acylantranilic acid was the starting-point. It will be seen upon examining the structure of the hypothetical intermediate product, the secondary amide, that the $-CO-NH-CO-$ group being symmetrical should be formed equally well from $RCN + R'.COOH$ as from $R'CN + R.COOH$; in other words, as the condensation takes place solely between the CN and $COOH$ it is immaterial which radical carries the CN and which the $COOH$. This same secondary amide should therefore result when acetylantranilic nitrile is heated with acetic acid.

RX(1) OF 1 A ==> B



RX(1) RCT A 25116-00-1
 RGT C 1310-58-3 KOH, D 7722-84-1 H2O2
 PRO B 1769-24-0
 SOL 7732-18-5 Water
 NTE Classification: Condensation; Heterocycle formation;
 Cyclisation; Hydration; # Conditions: KOH H2O2 H2O; 30-45 deg
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